UNITED STATES
ENVIRONMENTAL PROTECTION AGENCY (EPA)
HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM

ROBUST SUMMARIES DOSSIER
for MEMBERS of the HIGHER OLEFINS CATEGORY
CONTAINING C18 – C54 OLEFINS

Members containing C18-C54 olefins:

CAS No. 112-88-9, 1-Octadecene
CAS No. 3452-07-1, 1-Eicosene
CAS No. 1599-67-3, 1-Docosene
CAS No. 10192-32-2, 1-Tetracosene
CAS No. 68855-59-4; Alkenes, C14-18 alpha
CAS No. 68855-60-7; Alkenes, C14-20 alpha
CAS No. 93924-10-8, a-Olefin fraction C20-24 cut
CAS No. 93924-11-9, a-Olefin fraction C24-28 cut
CAS No. 131459-42-2; Alkene, C24-54 branched and linear, alpha
CAS No. 93762-80-2; Alkenes, C15-C18

Contains Robust Summaries for the Following Substances:

CAS No. 112-88-9, 1-Octadecene
CAS No. 27070-58-2, Octadecene
CAS No. 27070-58-2, Octadecenes; CAS No. 182636-02-8, Branched Octadecenes
C16/18 Internal Olefin Blend and C16/18 Alpha Olefin Blend
CAS No. 3452-07-1, 1-Eicosene; CAS No. 1599-67-3, 1-Docosene
CAS No. 10192-32-2, 1-Tetracosene; CAS No. 18835-33-1, 1-Hexacosene
CAS No. 18835-34-2, 1-Octacosene; CAS No. 18435-53-5, 1-Triacontene
Alpha Olefin Blends: C14-C18, C18-C24, C18-C26
CAS No. 93924-10-8, C20-24 Alpha Olefin
C20-24 Alkenes, Branched/Linear: CAS Nos. 182636-03-9, 182636-04-0, 182636-05-1
C24-30 Alkenes, Branched/Linear: CAS Nos. 182636-05-1, 182636-06-2, 182636-07-3, 182636-08-4
C54 Alpha Olefin; and CAS No. 131459-42-2; Alkene, C24-54, branched and linear, alpha

Prepared by:

American Chemistry Council
Higher Olefins Panel

April 28, 2005

1. GENERAL INFORMATION

1.01 Details on Chemical Category

The Higher Olefins Category consists of a non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins (C_6 through C_{54}) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. All CAS numbers are within the HPV Challenge Program. The $C_6 - C_{14}$ even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Panel sponsored the C_6, C_7, C_8, C_9, C_{10}, C_{12} and C_{10-13} aliphatic linear and branched internal olefins and the C_{16} and C_{18} aliphatic linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). The members of the category are presented in the following table.

Members of the Higher Olefins Category

Alpha Olefins	Branched/Linear	CAS No.
Neohexene	Branched	558-37-2
1-Tridecene	Linear	2437-56-1
1-Hexadecene (ICCA)	Linear	629-73-2
1-Octadecene (ICCA)	Linear	112-88-9
1-Eicosene	Linear	3452-07-1
1-Docosene	Linear	1599-67-3
1-Tetracosene	Linear	10192-32-2
Alkenes, C10-16 alpha	Linear	68855-58-3
Alkenes, C14-18 alpha	Linear	68855-59-4
Alkenes, C14-20 alpha	Linear	68855-60-7
a-Olefin fraction C20-24 cut	Linear	93924-10-8
a-Olefin fraction C24-28 cut	Branched and Linear	93924-11-9
Alkene, C24-54 branched and linear, alpha	Branched and Linear	131459-42-2
Internal Olefins		
Hexene (ICCA)	Linear	25264-93-1
Heptene (ICCA)	Linear	25339-56-4
Octene (ICCA)	Linear	25377-83-7
Nonene (ICCA)	Linear	27215-95-8
Dodecene (ICCA – not sponsored in HPV)	Linear	25378-22-7
Alkenes, C6	Branched and Linear	68526-52-3
Alkenes, C6-8, C7 rich	no data available	68526-53-4
Alkenes, C7-9, C8-rich	Linear	68526-54-5
Alkenes, C8-10, C9-rich	Linear	68526-55-6
Alkenes, C9-11, C10-rich	Linear	68526-56-7
Alkenes, C10-12, C11-rich	Linear	68526-57-8
Alkenes, C11-13, C12-rich	Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-10-8
Alkenes, C10-16	Linear	68991-52-6
Alkenes, C15-C18	Linear	93762-80-2
C10,12 Olefin rich hydrocarbons	Linear	68514-32-9
C12,14 Olefin rich hydrocarbons	Linear	68514-33-0

1.1 General Substance Information

A. Type of Substance

Element [ ]; Inorganic [ ]; Natural substance [ ]; Organic [X]; Organometallic [ ]; Petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

Gaseous [ ]; Liquid [X]; Solid [X]

Remarks: The C6-C16 members of the category are colorless liquids; C18 is a colorless liquid or white solid depending on ambient temperature; and C20-C54 members are white solids.

C. Purity:

C18 – C54 alpha olefins and C18 internal olefin are manufactured and marketed as components of blends. C18 – C24 alpha olefins are also manufactured and marketed as single carbon number products. The purity of 1-octadecene has been reported by manufacturers as 90.6% , as >91% and as 80-98%. The purities of the C20, C22, and C24 individual alpha olefins have been reported by manufacturers as 100%.

1.2 Impurities

Remark: The compositions reported by manufacturers for the members of the Higher Olefins Category containing C18-C54 olefins are shown below:

Alpha Olefins	CAS No.	Composition/Impurities
1-Octadecene	112-88-9	7.7% vinylidenes (branching at 2nd carbon), max. 5% C16 and lower olefins, max. 20% C20 and higher olefins
1-Eicosene	3452-07-1	C20 linear. No impurities or branching
1-Docosene	1599-67-3	C22 linear. No impurities or branching
1-Tetracosene	10192-32-2	C24 linear. No impurities or branching
Alkenes, C14-18 alpha	68855-59-4	Typical composition: 1% C12, 65% C14, 33% C16, 1% C18; 99.5% monoolefin; 0.5% paraffin; 82.0% linear terminal; 14% branched terminal; 4% linear internal
Alkenes, C14-20 alpha	68855-60-7	Typical composition: 1% C14, 57% C16, 37% C18, 5% C20; 99.2% monoolefin; 0.8% paraffin; 61.5% linear terminal; 32.5% branched terminal; 6% linear internal
a-Olefin fraction C20-24 cut	93924-10-8	Max. composition: 3% C18, 47% C20, 35% C22, 26% C24, 1% C26, 89.3% linear, 8.3% branched, 0.3% paraffin;

		Also reported: C18 = max.5%, C20 = 45-60%, C22 = 30-50%, C24 = max.15%, C26 = max.1%
a-Olefin fraction C24-28 cut	93924-11-9	Max. composition: 9% C24, 18% C26, 17% C28, 12% C30, 0.8% paraffin, 0.6% paraffin
Alkene, C24-54 branched and linear, alpha	131459-42-2	Max. 28% C28 and lower carbon number, min. 72% C30+ , 33-39% branched, >50% linear alpha olefin, 10% internal olefins
Internal Olefins		
Alkenes, C15-C18	93762-80-2	Mostly linear, less than 2% branched.

1.3 Additives

None

1.4 Synonyms

1.5 Quantity

Remarks: U.S. production volumes for C18 - C54 containing members of the Higher Olefins Category reported for 2002 by members of the American Chemistry Council's Higher Olefins Panel:

COMPOUND	CAS NUMBER	2002 PRODUCTION VOLUME (Million Pounds)
Alpha Olefins		
1-Octadecene (ICCA)	112-88-9	100-200
1-Eicosene	3452-07-1	50-100
1-Docosene	1599-67-3	50-100
1-Tetracosene	10192-32-2	10-50
Alkenes, C14-18 alpha	68855-59-4	1-10
Alkenes, C14-20 alpha	68855-60-7	50-100
a-Olefin fraction C20-24 cut	93924-10-8	50-100
a-Olefin fraction C24-28 cut	93924-11-9	100-200
Alkene, C24-54 branched and linear, alpha	131459-42-2	50-100
Internal Olefins		
Alkenes, C15-C18	93762-80-2	700-800

Reference: American Chemistry Council's Higher Olefins Panel (2002)

1.6 Use Pattern

A. General Use Pattern

Type of Use:

Category:

(a) Main Use in closed systems

Industrial Use: Chemical industry – chemicals used in synthesis Intermediate

Remarks:

CHAIN LENGTH	APPLICATION
C18-C20	Direct components of drilling fluids for off-shore oil exploration
C18	Intermediates in the production of lube oil additives, surfactants, hydraulic fluids and additives
C20-C24	Wax applications [e.g., candles, board/box coatings, polishes]; intermediates for lube oil additives, epoxides used for epoxy resins and polyurethanes, chlorinated plasticizers for PVC, fire retardant agents, additives for metal working fluids
C24-C28	Wax applications [e.g., candles, board/box coatings, polishes]; intermediates for lube oil additives, epoxides used for epoxy resins and polyurethanes, additives for metal working fluids
C24-C54	Wax applications [e.g., candles, board/box coatings, polishes]; intermediates for lube oil additives, additives for metal working fluids, lubricants for PVC extrusion

(b) Main Industrial Use: Non-dispersive use
Chemical industry – chemicals used in synthesis
Intermediate

Remarks: See entry for (a)

Reference: American Chemistry Council's Higher Olefins Panel (2002)

B. Uses In Consumer Products

C20-C54 alpha olefins may be used in wax applications (eg., candles, board/box coatings, polishes)

1.7 Sources of Exposure

Source:

Remarks: These products are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals. C_{18} to C_{20} olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. $C_{20} - C_{54}$ alpha olefins are used in wax applications. No other non-intermediate applications have been identified. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. It is a common practice to use personal protective equipment. In the case of dermal exposures, protective gloves would be worn with the C18 and lower molecular

weight chemicals due to the mildly irritating properties of these substances (ACC Higher Olefins Panel). Results from modelled data suggest that on-site waste treatment processes are expected to remove these substances from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge (EPIWIN, 2000). These substances are not on the US Toxic Release Inventory (TRI) list (NLM, 2003). These olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

Reference: American Chemistry Council's Higher Olefins Panel (2002)

1.8 Additional Information

A. Classification and Labelling

B. Occupational Exposure Limits

Exposure Limit Value

Type: None established
Value:

Short Term Exposure Limit Value

Value: None established

C. Options for Disposal

Remarks: Incineration or diversion to other hydrocarbon uses

D. Last Literature Search

Type of search: Internal and external
Date of search: October 2003
Remark: Medline
IUCLID
TSCATS
ChemIDplus
AQUIRE - ECOTOX

2. PHYSICAL CHEMICAL DATA

2.1 Melting Point

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Because the differences in results were large, the selected value was a weighted value rather than a mean value.

Results

Melting point value in °C:	17.70°C
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.
	EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed:	ASTM D 97
GLP:	No data
Year:	No data
Test Conditions:	In accord with ASTM D97

Results

Melting point value in °C:	18.3°C

Reliability:	(2) Reliable with restrictions. Reliable source. These data were not reviewed for quality.
Flag:	Key study for SIDS endpoint
References:	Chevron Phillips Chemical Company MSDS, The Woodlands, TX (unpublished report).

C. Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed:	No data
GLP:	No data
Year:	No data
Test Conditions:	No data

Results

Melting point value in °C:	17.5°C
Reliability:	(2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.
References:	EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity:	CAS No. 27070-58-2, Octadecene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where

Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. EPIWIN used the structure for 1-octadecene. Because the differences in results were large, the selected value was a weighted value rather than a mean value.

Results

Melting point value in °C: 29.57°C

Reliability: (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

E. Test Substance

Identity: CAS No. 3452-07-1, 1-Eicosene

Method

Method/ guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Melting point value in °C: 28.5°C

Reliability: (2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity:	CAS No. 1599-67-3, 1-Docosene

Method

Method/ guideline followed:	No data
GLP:	No data
Year:	No data
Test Conditions:	No data

Results

Melting point value in °C:	38°C
Reliability:	(2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.
Flag:	Key study for SIDS endpoint
References:	EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity:	CAS No. 10192-32-2, 1-Tetracosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.

Results

Melting point value in °C:	96.76°C
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity:	CAS No. 18835-33-1, 1-Hexacosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.

Results

Melting point value in °C:	114.81°C
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity: CAS No. 18835-34-2, 1-Octacosene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.

Results

Melting point value in °C: 132.85°C

Reliability: (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

J. Test Substance

Identity: CAS No. 18435-53-5, 1-Triacontene

Method

Method/
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.

Results

Melting point
value in °C: 150.90°C

Reliability: (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

K. Test Substance

Identity: C54 alpha olefin

Method

Method/
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Because the differences in results were large, the selected value was a weighted value rather than a mean value.

Results

Melting point value in °C:	319.14°C
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.2 Boiling Point

A. Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene or CAS 27070-58-2, Octadecene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Calculations for both substances used the structure for 1-octadecene.

Results

Boiling point value in °C:	306.27°C
Pressure:	
Pressure unit:	1013
Remarks:	hPa
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method/
guideline followed: No data
GLP: No data
Year: No data
Test Conditions: No data

Results

Boiling point
value in °C: 315°C
Pressure: 1013
Pressure unit: hPa
Remarks:

Reliability: (2) Reliable without restrictions. Reliable secondary source. Data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: Texas Research Center Thermodynamics Tables, Texas A&M University, College Station, Texas, USA.

C. Test Substance

Identity: CAS No. 3452-07-1, 1-Eicosene

Method

Method/
guideline followed: No data
GLP: No data
Year: No data
Test Conditions: No data

Results

Boiling point	
value in °C:	341°C
Pressure:	1013
Pressure unit:	hPa
Remarks:	

Reliability: (2) Reliable with restrictions. Experimental result as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity: CAS No. 1599-67-3, 1-Docosene

Method

Method/	
guideline followed:	No data
GLP:	No data
Year:	No data
Test Conditions:	No data

Results

Boiling point	
value in °C:	367°C
Pressure:	1013
Pressure unit:	hPa
Remarks:	

Reliability: (2) Reliable with restrictions. Experimental result as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

E. Test Substance

Identity: CAS No. 10192-32-2, 1-Tetracosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994).

Results

Boiling point value in °C:	379.97°C
Pressure:	
Pressure unit:	1013
Remarks:	hPa
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587. EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity:	CAS No. 18835-33-1, 1-Hexacosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994).

Results

Boiling point value in °C:	403.17°C
Pressure:	

Pressure unit:	1013
Remarks:	hPa
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587. EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity:	CAS No. 18835-34-2, 1-Octacosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994).

Results

Boiling point value in °C:	426.38°C
Pressure:	
Pressure unit:	1013
Remarks:	hPa
Reliability:	(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity: CAS No. 18435-53-5, 1-Triacontene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994).

Results

Boiling point value in °C: 449.59°C

Pressure:

Pressure unit: 1013

Remarks: hPa

Reliability: (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity: C54 alpha olefin

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN MPBPWIN v 1.41

GLP:	Not applicable
Year:	Not applicable

Test Conditions: Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994).

Results

Boiling point value in °C:	728.08°C
Pressure:	
Pressure unit:	1013
Remarks:	hPa

Reliability: (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.3 Density (Relative Density)

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Remarks: Purity approx. 92%

Method

Method:	ASTM D 287
GLP:	No

Test Conditions: No data

Results

Type: Bulk density [ ]; Density [ ]; Relative Density [x]

Value: 0.793

Temperature (°C): 15.6/15.6

Reliability: (2) Reliable with restrictions. Test conducted by reliable testing facility but data were not evaluated for quality.

Reference: Chevron Phillips Chemical Company, The Woodlands, TX (unpublished report).

B. Test Substance

Identity: CAS No. 3452-07-1, 1-Eicosene

Method

Method: No data
GLP: No

Test Conditions: Calculated

Results

Type: Bulk density [ ]; Density [ ]; Relative Density [x]

Value: 0.79

Temperature (°C): 30

Reliability: (2) Reliable with restrictions. Value is calculated data from a reliable source, but method used for calculation was not available for review.

Reference: Shell Chemical LP, Houston, TX.

C. Test Substance

Identity: CAS No. 1599-67-3, 1-Docosene

Method

Method: No data
GLP: No

Test Conditions: Calculated

Results

Type: Bulk density [ ]; Density [ ]; Relative Density [x]

Value: 0.79

Temperature (°C): 30

Reliability:	(2) Reliable with restrictions. Value is calculated data from a reliable source, but method used for calculation was not available for review.
Reference:	Shell Chemical LP, Houston, TX.

D. Test Substance

Identity:	CAS No. 10192-32-2, 1-Tetracosene

Method

Method:	No data
GLP:	No
Test Conditions:	Calculated

Results

Type:	Bulk density [ ]; Density [ ]; Relative Density [x]
Value:	0.79
Temperature (°C):	30
Reliability:	(2) Reliable with restrictions. Value is calculated data from a reliable source, but method used for calculation was not available for review.
Reference:	Shell Chemical LP, Houston, TX.

2.4 Vapour Pressure

A. Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed:	Not reported
GLP:	Not applicable
Year:	
Test Conditions:	

Results

Vapor Pressure value:	0.00009 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.0000675 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: Daubert, T.E. and Danner, R.P. (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation; Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Pub. Corp., New York, NY; EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP: Not applicable
Year: Not applicable

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an experimental value for BP of 315 °C.

Results

Vapor Pressure value: 0.00223 hPa
Temperature (°C): 25°C
Remarks: Reported as 0.00167 mm Hg

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

References: Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed:	Calculated value using NOMO5 method using two measured values at higher temperature and reduced boiling points.
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	No data

Results

Vapor Pressure value:	0.00085 – 0.0013 hPa
Temperature (°C):	25°C
Reliability:	(2) Reliable with restrictions. The result is calculated data.
References:	U.S. Environmental Protection Agency, Review by Dr. L. Scarano, OPPT/Risk Assessment Division.

D. Test Substance

Identity:	CAS No. 27070-58-2, Octadecene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an estimated (EPIWIN, 2000) value for BP of 306.27 °C. The boiling point calculation used the structure for 1-octadecene.

Results

Vapor Pressure value:	0.0035 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.00261 mm Hg
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag:	Key study for SIDS endpoint
References:	Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press. EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

E. Test Substance

Identity:	CAS No. 3452-07-1, 1-Eicosene
Method	
Method/ guideline followed:	Not reported
GLP:	Not applicable
Year:	
Test Conditions:	Results were extrapolated from measured values
Results	
Vapor Pressure value:	0.000014 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.0000106 mm Hg (25°C)
Reliability:	(2) Reliable with restrictions. The result is extrapolated data as cited in the EPIWIN database. These data were not reviewed for quality.
Flag:	Key study for SIDS endpoint
References:	Yaws CL (1994). as cited in EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity:	CAS No. 3452-07-1, 1-Eicosene
Method	
Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable

Year:	Not applicable
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an experimental value for BP of 341 °C and an experimental value for melting point of 28.5 °C .

Results

Vapor Pressure value:	0.000545 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.000409 mm Hg
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.
References:	Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press. EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity:	CAS No. 1599-67-3, 1-Docosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used experimental values of 367 °C for boiling point and 38°C for melting point.

Results

Vapor Pressure value:	0.000115 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.0000864 mm Hg

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity: CAS No. 10192-32-2, 1-Tetracosene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an estimated (EPIWIN, 2000) value for BP of 379.97 °C and an estimated melting point of 96.76 °C .

Results

Vapor Pressure value: 0.00001533 hPa

Temperature (°C): 25°C

Remarks: Reported as 0.0000115 mm Hg

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity:	CAS No. 18835-33-1, 1-Hexacosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an estimated (EPIWIN, 2000) value for BP of 403.17 °C and an estimated melting point of 114.81 °C .

Results

Vapor Pressure value:	0.00000288 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.00000216 mm Hg
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press. EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

J. Test Substance

Identity:	CAS No. 18835-34-2, 1-Octacosene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an estimated (EPIWIN, 2000) value for BP of 426.38 °C and an estimated melting point of 132.85 °C .

Results

Vapor Pressure value:	0.000000529 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.000000397 mm Hg
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press. EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

K. Test Substance

Identity:	CAS No. 18435-53-5, 1-Triacontene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an estimated (EPIWIN, 2000) value for BP of 449.59 °C and an estimated melting point of 150.90 °C .

Results

Vapor Pressure value:	9.4 [E-8] hPa
Temperature (°C):	25°C
Remarks:	Reported as 7.12[E-8] mm Hg
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint

References: Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

L. Test Substance

Identity: C54 alpha olefin

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41
GLP: Not applicable
Year: Not applicable

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. The calculation used an estimated (EPIWIN, 2000) value for BP of 728.08 °C and an estimated melting point of 319.14 °C .

Results

Vapor Pressure value: 1.1319[E-16] hPa
Temperature (°C): 25°C
Remarks: Reported as 8.49[E-17] mm Hg

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.5 Partition Coefficient (log10Kow)

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method:	OECD Guideline 117
GLP:	Yes
Year:	1985

Test Conditions: Reverse phase HPLC method was employed for measuring the partition coefficients. The HPLC system used was a reverse-phase C18-coated silica gel column (Partisil ODS-3), 250 mm x 5 mm id, with a mobile phase of 19 volumes methanol and 1 volume water (final pH 6.8) at a flow rate of 1 ml min-1. Samples of an approximate 1 mg ml-1 solution in the above mobile phase were injected and the emergence of the material detected using relative index detection. From the retention time of the peak, the log Kow value was determined.

Results

Log Kow:	>8
Temperature (°C):	25

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

Reference: Pearson, N. (1985) Shell Research Ltd. Report SBGR.85.059. Reported in IUCLID.

B. Test Substance

Identity: C18-54 alpha olefins and C18 internal olefin

Method

Method:	Calculated value using the computer program EPIWIN, KOWWIN v1.67
GLP:	Not applicable
Year:	Not applicable

Test Conditions: Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995).

Results

Substance	CAS NUMBER	Log Kow
1-Octadecene	112-88-9	9.04
Octadecene	27070-58-2	9.04
1-Eicosene	3452-07-1	10.03
1-Docosene	1599-67-3	11.01
1-Tetracosene	10192-32-2	11.99
1-Hexacosene	18835-33-1	12.97
1-Octacosene	18835-34-2	13.96
1-Triacontene	18435-53-5	14.94
C54 Alpha Olefin	--	26.72

Reliability: (2) Reliable with restrictions. The results were calculated based on chemical structure as modeled by EIPWIN.

Flag: Key study for SIDS endpoint

Reference: Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.6.1 Water Solubility (including *Dissociation Constant).

A. Test Substance

Identity: C18 – C54 alpha olefins and C18 internal olefin

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN, WSKOW v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used values for Log Kow (estimated

by EPIWIN) and measured values (from EPIWIN database) for melting point, when the values were available.

Results

Substance	CAS NUMBER	Log Kow used	Melting Point used (°C)	Water Solubility (mg/L)
1-Octadecene	112-88-9	9.04	18.3	1.508 [E-4]
Octadecene	27070-58-2	9.04	--	1.256 [E-4]
1-Eicosene	3452-07-1	10.03	--	1.264 [E-5]
1-Docosene	1599-67-3	11.01	--	1.259 [E-6]
1-Tetracosene	10192-32-2	11.99	--	1.244 [E-7]
1-Hexacosene	18835-33-1	12.97	--	1.22 [E-8]
1-Octacosene	18835-34-2	13.96	--	1.19 [E-9]
1-Triacontene	18435-53-5	14.94	--	1.155 [E-10]
C54 Alpha Olefin	--	26.72	--	6.33 [E-23]

Reliability: (2) Reliable with restrictions. The results were calculated by EPIWIN using an estimated Log Kow.

Flag: Key study for SIDS endpoint

References:

Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN, WATERNT v 1.01

GLP:	Not applicable
Year:	Not applicable
Test Conditions:	The water solubility is calculated by the WATERNT subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995).
Results	
Value(mg/L) at temperature (°C):	3.793E-005 mg/L (25°C)
Reliability:	(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EPIWIN.
References:	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92. EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.6.2 Surface tension

No data

2.7 Flash Point (Liquids)

Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method: ASTM D93
GLP: No data

Test Conditions: No data

Results

Value (°C): 154 °C
Type of test: Pensky-Martens closed cup tester

Reliability: (2) Reliable with restrictions. Test conducted by reliable testing facility but data were not evaluated for quality.

Reference: Chevron Phillips Chemical Company Product Brochure, Company test results, Chevron Phillips Chemical Company, The Woodlands, TX.

2.8 Auto Flammability (Solids/Gases)

Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method: No data
GLP: No

Test Conditions: No data

Results

Value (°C): 250 °C
Pressure (hPa): No data

Reliability: (2) Reliable with restrictions. Test conducted by reliable testing facility but data were not evaluated for quality.

Reference: Chevron Phillips Chemical Company Product Brochure, Company test results, Chevron Phillips Chemical Company, The Woodlands, TX.

2.9 Flammability

Result: Non flammable
Method: Defined by flash point

2.10 Explosive Properties

Result: Not explosive
Method: Based on thermodynamic information

2.11 Oxidising Properties

Result: No oxidizing properties
Method: Based on structural formula

2.12 Oxidation-Reduction Potential

Not applicable

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 Stability

A. Photodegradation

(1) Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene CAS No. 3452-07-1, 1-Eicosene CAS No. 1599-67-3, 1-Docosene CAS No. 10192-32-2, 1-Tetracosene CAS No. 68855-59-4; Alkenes, C14-18 alpha CAS No. 68855-60-7; Alkenes, C14-20 alpha CAS No. 93924-10-8, a-Olefin fraction C20-24 cut CAS No. 93924-11-9, a-Olefin fraction C24-28 cut CAS No. 131459-42-2; Alkene, C24-54 branched/linear, alpha CAS No. 93762-80-2; Alkenes, C15-C18

Method

Method/ guideline followed:	Other: Technical discussion
Type:	water
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Not applicable

Results

Direct photolysis:	In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Higher Olefins Category.
Remarks:	The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982a). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state. The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982a). Higher wavelengths (e.g. infrared) result only in

vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Olefins with one double bond, such as the chemicals in the Higher Olefins category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerization about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (Harris, 1982a).

Products in the Higher Olefins Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

Reliability: Not applicable

References:

Harris J C (1982a). Rate of Aqueous Photolysis. Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline (1977). Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

(2) Test Substance

Identity: C18-54 alpha olefins and C18 internal olefin

Method

Method/
guideline followed: Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11, which uses a

program described by Meylan and Howard, 1993. EPIWIN used the alpha olefin structures for the calculations.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Substance	Sensitiser (type): OH		Sensitiser (type) Ozone	
	Rate Constant (cm^3/molecule-sec)	Hours to reach 50% degradation using a 12-hr day and avg. OH conc. of 1.5 E6 OH/cm^3	Rate Constant (cm^3/molecule-sec)	Hours to reach 50% degradation using avg. ozone conc. of 7 E11 mol/cm^3
1-Octadecene	47.1346 E-12	2.7	1.2 E-17	22.9
Octadecene	47.1346 E-12	2.7	1.2 E-17	22.9
1-Eicosene	49.9606 E-12	2.6	1.2 E-17	22.9
1-Docosene	52.7867 E-12	2.4	1.2 E-17	22.9
1-Tetracosene	55.6128 E-12	2.3	1.2 E-17	22.9
1-Hexacosene	58.4389 E-12	2.2	1.2 E-17	22.9
1-Octacosene	61.2650 E-12	2.1	1.2 E-17	22.9
1-Triacontene	64.0911 E-12	2.0	1.2 E-17	22.9
C54 Alpha Olefin	98.0043 E-12	1.3	1.2 E-17	22.9

Reliability: (2) Reliable with restrictions. The values were calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.

Flag: Critical study for SIDS endpoint

References:

Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 26: 2293-99

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Stability in Water

Test Substance

Identity:

CAS No. 112-88-9, 1-Octadecene
CAS No. 3452-07-1, 1-Eicosene
CAS No. 1599-67-3, 1-Docosene
CAS No. 10192-32-2, 1-Tetracosene
CAS No. 68855-59-4; Alkenes, C14-18 alpha
CAS No. 68855-60-7; Alkenes, C14-20 alpha
CAS No. 93924-10-8, a-Olefin fraction C20-24 cut
CAS No. 93924-11-9, a-Olefin fraction C24-28 cut
CAS No. 131459-42-2; Alkene, C24-54 branched/linear, alpha
CAS No. 93762-80-2; Alkenes, C15-C18

Method

Method/
guideline followed: Other – Technical Discussion

Test Conditions: Not applicable

Results: Not applicable

Remarks: Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (Harris, 1982b) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Higher Olefins Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

The substances in the Higher Olefins Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Higher Olefins Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

Conclusions: In the environment, hydrolysis will not contribute to the degradation of the C18-C54 alpha or C18 internal olefins.

Reliability: Not applicable

References:

Gould, E.S. (1959) Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982b) "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W. B. (1985) Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

C. Stability In Soil

No data available

3.2 Monitoring Data (Environment)

No data available.

3.3 Transport and Distribution

3.3.1 Transport between environmental compartments

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	252
Water solubility:	0.0001508 g/m^3
Vapor pressure:	0.009 Pa (25°C)
Log Kow:	9.04
Melting point:	18.3°C

Half-life in air = 4.4 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	<1%	<1%
Water	<1%	7.9%
Soil	97.5%	22.3%
Sediment	2.2%	69.6%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that 1-octadecene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 27070-58-2, Octadecene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	252
Water solubility:	0.000126 g/m^3
Vapor pressure:	0.350 Pa (25°C)
Log Kow:	9.04
Melting point:	29.6°C

Half-life in air = 4.4 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	12.5%	<1%
Water	<1%	7.9%
Soil	85.5%	22.2%
Sediment	1.9%	69.7%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that octadecene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity: CAS No. 3452-07-1, 1-Eicosene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	280.54
Water solubility:	0.0000126 g/m^3
Vapor pressure:	0.00141 Pa (25°C)
Log Kow:	10.03
Melting point:	28.5°C

Half-life in air = 4.2 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	<1%	<1%
Water	<1%	7.8%
Soil	97.7%	22.4%
Sediment	2.2%	69.5%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that 1-eicosene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity: CAS No. 1599-67-3, 1-Docosene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	308.6
Water solubility:	0.00000126 g/m^3
Vapor pressure:	0.0115 Pa (25°C)
Log Kow:	11.0
Melting point:	38°C

Half-life in air = 4.01 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	<1%	<1%
Water	<1%	7.9%
Soil	97.2%	22.2%
Sediment	2.2%	69.7%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that 1-docosene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

E. Test Substance

Identity: CAS No. 10192-32-2, 1-Tetracosene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	336.65
Water solubility:	0.000000124 g/m^3
Vapor pressure:	0.00153 Pa (25°C)
Log Kow:	11.99
Melting point:	96.76°C

Half-life in air = 3.84 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	Level III
Air	<1%	<1%

Water	<1%	7.9%
Soil	97.7%	22.3%
Sediment	2.2%	69.7%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that 1-tetracosene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 18835-33-1, 1-Hexacosene

Method

Type: Fugacity model, Mackay Level III

Remarks: EPIWIN Level III Fugacity Model used for calculations (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	364.7
Henry's LC:	104 atm-m3/mole
Vapor pressure:	2.16 E-6 mm Hg (25°C)
Log Kow:	13
Melting point:	115°C
Soil Koc:	3.83 E12

Half-life in air = 3.69 hr, half-life in water = 900 hr, half-life in soil = 900 hr, half-life in sediment = 3600 hr
Environment name: EQC Standard Environment

All other parameters were default values. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	Nda	<1%
Water	Nda	3.5%
Soil	Nda	27.2%
Sediment	Nda	69.2%

Remarks: Level I was not performed because the Trent University Level I model did not appear to be suitable for this substance and the EPIWIN Suite does not include Level I. Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: Level I was not performed. These results indicated that 1-hexacosene will partition primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity: CAS No. 18835-34-2, 1-Octacosene

Method

Type: Fugacity model, Mackay Level III

Remarks: EPIWIN Level III Fugacity Model used for calculations (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	392.76
Henry's LC:	183 atm-m3/mole
Vapor pressure:	3.97 E-7 mm Hg (25°C)
Log Kow:	14

Melting point: 133°C
Soil Koc: 3.74 E13

Half-life in air = 3.54 hr, half-life in water = 900 hr, half-life in soil = 900 hr, half-life in sediment = 3600 hr
Environment name: EQC Standard Environment

All other parameters were default values. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	Nda	<1%
Water	Nda	3.5%
Soil	Nda	27.5%
Sediment	Nda	68.9%

Remarks: Level I was not performed because the Trent University Level I model did not appear to be suitable for this substance and the EPIWIN Suite does not include Level I. Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: Level I was not performed. These results indicated that 1-octacosene will partition primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity: CAS No. 18435-53-5, 1-Triacontene

Method

Type: Fugacity model, Mackay Level III

Remarks: EPIWIN Level III Fugacity Model used for calculations (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	420.81
Henry's LC:	322 atm-m3/mole
Vapor pressure:	7.12 E-8 mm Hg (25°C)
Log Kow:	14.9
Melting point:	151°C
Soil Koc:	3.57 E14

Half-life in air = 3.41 hr, half-life in water = 900 hr, half-life in soil = 900 hr, half-life in sediment = 3600 hr
Environment name: EQC Standard Environment

All other parameters were default values. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	Nda	<1%
Water	Nda	3.4%
Soil	Nda	28%
Sediment	Nda	68.5%

Remarks: Level I was not performed because the Trent University Level I model did not appear to be suitable for this substance and the EPIWIN Suite does not include Level I. Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: Level I was not performed. These results indicated that 1-triacontene will partition primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity: C54 Alpha Olefin

Method

Type: Fugacity model, Mackay Level III

Remarks: EPIWIN Level III Fugacity Model used for calculations (EPIWIN, 2000)

Chemical assumptions:

Molecular weight:	757.46
Henry's LC:	2.89 E5 atm-m3/mole
Vapor pressure:	8.49 E-17 mm Hg (25°C)
Log Kow:	26.7
Melting point:	319°C
Soil Koc:	2.15 E26

Half-life in air = 2.35 hr, half-life in water = 1440 hr, half-life in soil = 1440 hr, half-life in sediment = 5760 hr
Environment name: EQC Standard Environment

All other parameters were default values. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	Nda	<1%
Water	Nda	2.4%
Soil	Nda	29.2%
Sediment	Nda	68.4%

Remarks: Level I was not performed because the Trent University Level I model did not appear to be suitable for this substance and the EPIWIN Suite does not include Level I. Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: Level I was not performed. These results indicated that C54 alpha olefin will partition primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

J. Test Substance

Identity: C18-C54 alpha olefins and C18 internal olefin

Method

Type: Volatilization from water

Remarks: Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant (estimated by Bond SAR method using HENRYWIN program) and EPIWIN default values.

Results:

Substance	CAS NUMBER	Henry's Law Constant (atm-m³/mole)	Half-life from Model River (hours)	Half-life from Model Lake (days)
1-Octadecene	112-88-9	10.7	1.6	6.3
Octadecene	27070-58-2	10.7	1.6	6.3
1-Eicosene	3452-07-1	18.9	1.7	6.6
1-Docosene	1599-67-3	33.4	1.8	7.0
1-Tetracosene	10192-32-2	58.8	1.9	7.3
1-Hexacosene	18835-33-1	104	1.9	7.6
1-Octacosene	18835-34-2	183	2.0	7.8
1-Triacontene	18435-53-5	322	2.1	8.1
C54 Alpha Olefin	--	2.89 [E5]	2.8	10.89

Reliability: (2) Valid with restrictions. Values are calculated.

References: EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.3.2 Distribution

A. Test Substance

Identity: C18-C54 alpha olefins and C18 internal olefin

Method

Method: Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66, based on the method of Meylan et al., 1992.

Test Conditions: Based on chemical structure. Program used the structure for alpha olefins.

Results

Value: Estimated Koc

Substance	CAS NUMBER	Estimated Koc
1-Octadecene	112-88-9	2.308 [E5]
Octadecene	27070-58-2	2.308 [E5]
1-Eicosene	3452-07-1	7.852 [E5]
1-Docosene	1599-67-3	2.671 [E6]
1-Tetracosene	10192-32-2	9.086 [E6]
1-Hexacosene	18835-33-1	3.091 [E7]
1-Octacosene	18835-34-2	1.051 [E8]
1-Triacontene	18435-53-5	3.577 [E8]
C54 Alpha Olefin	--	1.0 [E10]

Reliability: (2) Reliable with restrictions. Value is calculated.

Reference: EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: C18-54 alpha olefins and C18 internal olefin

Method

Method: Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.10

Test Conditions: Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values for vapor pressure (VP) and water solubility (WS) .

Results

Value: Henry's Law Constant (HLC)

Substance	Vapor Pressure used (mm Hg)	Water Solubility used (mg/L)	HLC Bond Estimate (atm-m^3/mole)	HLC Group Estimate (atm-m^3/mole)	HLC VP/Wsol Estimate (atm-m^3/mole)
1-Octadecene	6.75 [E-5]	1.51 [E-4]	10.7	33.8	0.1487
Octadecene	0.00261	1.26 [E-4]	10.7	33.8	6.904
1-Eicosene	4.09 [E-4]	1.26 [-5]	18.9	67.4	11.94
1-Docosene	8.64 [E-5]	1.26 [E-6]	33.4	134	27.87
1-Tetracosene	1.15 [E-5]	1.24 [E-7]	58.8	268	40.95
1-Hexacosene	2.16 [E-6]	1.22 [E-8]	104	535	84.96
1-Octacosene	3.97 [E-7]	1.19 [E-9]	183	1070	172.4
1-Triacontene	7.12 [E-8]	1.16 [E-10]	322	2130	341.3
C54 Alpha Olefin	1 [E-15]	6.33 [E-23]	2.89 [E5]	8.48 [E6]	1.574 [E7]

Reliability: (2) Reliable with restrictions. Values are calculated.

Reference: EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.4 Aerobic Biodegradation

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene (97.2%)

Remarks: Source: Shell Chemicals UK Ltd., Stanlow. Purity - 97.2%. Stability during use confirmed by infra-red spectra. Density - 0.788 kg/L @ 20°C. Clear, colorless liquid.

Method

Method/guideline: EEC Directive 84/449/EEC; Similar to OECD (301B) Modified Sturm Test
Type: Aerobic [X] Anaerobic [ ]
GLP: Yes
Year: 1985
Contact time: 41 days
Inoculum: Activated sludge

Test Conditions: Microorganisms were obtained from a fresh activated sludge from Canterbury Sewage Works (UK) according to standard test protocols. Test substance added to the test medium from a stock solution containing 2.4 g/L emulsified Dobane PT sulphonate. The final targeted nominal test concentration was 20 mg 1-Octadecene/L. Test medium was dispensed into Sturm vessels, inoculated, then aerated with 60 ml/min of CO_2-free air. Vessels were incubated at 22±1°C for 41 days. The extent of biodegradation was determined by titrating the total CO_2 released from the incubation on days 5, 7, 13, 16, 23, 28, 36, and 41. The medium was acidified on day 40 to release the total carbon dioxide by day 41. Controls with mineral medium and microbial innoculum (blank) were included.

Results: In the Modified Sturm Test, C18 linear alpha olefin was degraded with 77-81% of the theoretical amount of carbon dioxide being released in 28 days and 80-83% after 41 days. Although 1-Octadecene was biodegradable, 60% degradation was not reached within 10 days, which is required by the test guideline for "ready biodegradability."

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint

Reference: Cook K. (1985) C18 Linear Alpha Olefin: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center. Shell Report # SBGR.85.115 (unpublished report).

B. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene (97.2%)

Remarks: Source: Shell Chemicals UK Ltd., Stanlow. Purity - 97.2%. Stability during use confirmed by infra-red spectra. Density - 0.788 kg/L @ 20°C. Clear, colorless liquid.

Method

Method/guideline: EEC Directive 84/449/EEC; Similar to OECD (301D) Closed Bottle Test
Type: Aerobic [X] Anaerobic [ ]
GLP: Yes
Year: 1985
Contact time: *28* days
Inoculum: Activated sludge

Test Conditions: Microorganisms were obtained from Sittingbourne Sewage Works (UK) and prepared according to standard test protocols. Test substance added to the test medium from a stock solution containing 2.4 g/L emulsified Dobane PT sulphonate. The final test concentration was 3 mg 1-Octadecene/L. Test bottles were incubated at 21±1°C and the extent of biodegradation was determined by measuring oxygen concentration in the bottles at days 5, 15, and 28. Controls with no microbial innoculum

(control) and with medium plus microbial innoculum only (blank) were included. Sodium benzoate was used as a biodegradable substance to demonstrate the activity of the microbial innoculum.

Results: Under these conditions, 1-Octadecene was oxidized to 10-41% of the theoretical oxygen demand by day 5 and 39-48% by day 28. There was no significant inhibition of microbial activity under the test conditions. These results indicated that, although biodegradation occurred, 1-Octadecene was not considered readily biodegradable.

Reliability: (1) Reliable without restrictions

Reference: Cook K. (1985) C18 Linear Alpha Olefin: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center. Shell Report # SBGR.85.115 (unpublished report).

C. Test Substance

Identity: CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

Method

Method/guideline:	ISO "Marine BODIS" ISO/TC 147/SC 5/WG 4N 1415
Type:	Aerobic [X] Anaerobic [ ]
GLP:	No
Year:	1995
Contact time:	28 days
Inoculum:	None

Test Conditions: This method used natural seawater fortified with mineral nutrients and no inoculum was added in addition to the microorganisms already present in the seawater.

The test vessels were closed glass bottles with a known volume of aqueous test mixture (66.6%) and air (33.3%). They were shaken continuously to assure steady state oxygen partitioning between the aqueous and gaseous phase. The degradation was followed by weekly measurements of the BOD in the aqueous phase for a 28-day period. The test vessels were re-aerated and resealed after measurement. The total oxygen uptake in the test flasks was calculated from the measured oxygen concentration divided by the saturation value at normal conditions and multiplied with the total oxygen content originally present in the aqueous and gaseous phases.

Three replicates were used for each test condition: test substance, controls, and insoluble reference substance. The total oxygen capacity of each test vessel was 26.64 mg oxygen. Sodium benzoate was used as the soluble reference substance at a concentration of 20 mg of theoretical

oxygen demand (ThOD) per test vessel.

An inert support medium, chromatography silica powder, was used to provide a large and controlled surface area for the poorly-soluble test substance and reference substance (an olefin oil) The silica powder and test material were made into a homogenate and added to the test vessel before addition of the test medium. One gram of support medium containing 20 mg of ThOD of test substance or insoluble reference substance was used for each test vessel. The ThOD for the test substance was 0.34 mg oxygen/mg and the addition rate was 4 mg/test vessel.

The following controls were included: Background oxygen consumption in test medium, background oxygen consumption in test medium with clean silica powder.

Validity criteria stated: Temperature = 19-21°C, soluble reference is >60% in 14 days, and cumulative blank oxygen consumption is <30% of oxygen initially available. The reference insoluble material is expected to achieve 25-45% in 28 days.

Results: The test material achieved 48% biodegradation in 28 days.

Kinetic of Test substance:
7 day = 19 %
14 day = 31 %
21 day = 44 %
28 day = 48 %

Kinetic of control Substance (Sodium benzoate):
14 day = 58 %
28 day = 85 %

Reliability: (2) Reliable with restrictions: This study does not meet the validity criteria stated in the report. The soluble reference, sodium benzoate, only achieved 58% degradation by Day 14, instead of 60%.

Reference: Environment & Resource Technology Ltd. (1999) Assessment of ready aerobic degradability of C16/C18 isomerized olefin base fluid in seawater. Study No. 074-9. Conducted for Chevron Chemical Company (unpublished report).

D. Test Substance

Identity: CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 301B Modified Sturm Test (CO_2 evolution)
Type:	Aerobic [X] Anaerobic [ ]
GLP:	Yes
Year:	1998
Contact time:	28 days
Inoculum:	Sewage sludge, predominantly domestic
Concentration:	10 mg/L related to DOC (Dissolved Organic Carbon) 11.6 mg/L related to test substance
Statistical methods:	Not available

Test Conditions: A study was performed to assess the ready biodegradability of the test material in an aerobic aqueous medium. Approximately 24 hours prior to addition of the test and standard materials the vessels were filled with culture medium and inoculum (30 mg suspended solids/L), and aerated overnight. Test medium consisted of distilled water and mineral salts (phosphate buffer, ferric chloride).

Test vessels were sealed 5 L glass flasks containing 3 L of solution and CO2-free air bubbled through the solution at a rate of approximately 40 mL/min and stirred continuously by magnetic stirrer.

Test material was prepared by direct dispersion in culture media and tested in triplicate. Control and standard material (sodium benzoate) in were tested in duplicate. The test material was exposed to sewage sludge microorganisms at a concentration of 10 mg C/L with culture medium in sealed culture vessels in the dark at 21°C for 28 days. The standard material (sodium benzoate) concentration was also 10 mg C/L. Auxiliary solvents or surfactants were not used to aid or enhance solubility. Samples were taken on days 0, 1, 2, 3, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 27, 28 and 29.

The degradation of the test material was assessed by the determination of carbon dioxide produced. CO2 was measured by injecting samples into the inorganic carbon channel of the TOC analyzer.

The validation criteria for this study were:

The standard material yields >=60% degradation by day 14.

The test material may be considered to be readily biodegradable if >=60% degradation is attained after 28 days. This level of degradation must be reached within 10 days of biodegradation exceeding 10%.

The toxicity control should attain >=25% degradation by day 14 for the test material to be considered as non-inhibitory.

The difference of the extremes of replicate values of production of CO2 at the end of the test is less than 20%.

The total CO2 evolution in the control vessels at the end of the test

should not normally exceed 40 mg/L medium.

The Inorganic Carbon content of the test material in the culture media must be less than 5% of the Total Carbon on day 0.

Results

Degradation %:	92% after 28 days
Results:	Readily biodegradable
Kinetic of Test substance:	1 day = 4% 3 day = 15% 10 day = 53% 16 day = 83% 28 day = 92%
Control substance:	Benzoic acid, sodium salt
Kinetic:	14 day = 96% 28 day = 100%
Breakdown Product:	not measured
Remarks:	The test material attained a total of 92% degradation after 28 days and met the 10-day window validation criterion whereby greater than 60% degradation must be attained within 10 days of the degradation exceeding 10%. Toxicity control attained 100% degradation after 28 days confirming that the test material was not toxic to sewage treatment microorganisms used in the study. All validity criteria required were achieved; therefore, C20-24 Alkenes, Branched and Linear can be considered to be readily biodegradable under the strict terms and conditions of OECD Guideline No. 301B.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
Reference:	Handley, JW and Mead C (1998). C20-24 alkenes, branched and linear: Assessment of Ready Biodegradability; CO2 Evolution Test, Project No. 703/127. Conducted for Chevron Research and Technology Company (unpublished report).

E. Test Substance

Identity: C18, C22, C24, C26, C28, C30, C54 alpha olefins; C18 internal olefin

Method

Method/guideline: Estimated using the computer program EPIWIN v 3.10, BIOWIN v 4.00
Type: Aerobic

Test Conditions: Estimates use methods described by Howard et al., 1992; Boethling et al., 1994; and Tunkel et al., 2000. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

Results: Linear model prediction: Biodegrades fast [all except C54]
Non-linear model prediction: Biodegrades fast [C18 - C24]
Does not biodegrade fast [C26+]

Ultimate biodegradation timeframe: Weeks [C18 - C24]
Weeks-Months [C26,C28, C30]
Months [C54]

Primary biodegradation timeframe: Days [C18]
Days-Weeks [C20-C30]
Weeks [C54]
MITI linear model prediction: Biodegrades fast [all]
MITI non-linear model prediction: Biodegrades fast [all]

Reliability: (2) Reliable with restriction: Results are estimated

Reference: Boethling, R.S., P.H. Howard, W. Meylan, W. Stiteler, J. Beaumann and N. Tirado (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ. Sci. Technol. 28:459-65.

Howard, P.H., R.S. Boethling, W.M. Stiteler, W.M. Meylan, A.E. Hueber, J.A. Beauman and M.E. Larosche (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ. Toxicol. Chem. 11:593-603.

Tunkel, J. P.H. Howard, R.S. Boethling, W. Stiteler and H. Loonen (2000) Predicting ready biodegradability in the MITI Test. Environ. Toxicol. Chem. (accepted for publication)

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS Nos. C24=182636-05-1, C26=182636-06-2, C28=182636-07-3, C30=182636-08-4: C24-30 Alkenes, Branched and Linear

Remarks: even-numbered carbons only (<55% C24, <40% C26, <15% C28, <30% C30; 70% branched)

Method

Method/guideline:	OECD 301B Modified Sturm Test (CO_2 evolution)
Type:	Aerobic [X] Anaerobic [ ]
GLP:	Yes
Year:	2000
Contact time:	28 days
Inoculum:	Sewage sludge, predominantly domestic
Concentration:	10 mg/L related to DOC (Dissolved Organic Carbon) 17.1 mg/L related to test substance
Dilution water Chemistry:	Reagents recommended in the OECD guidelines were dissolved in deionized and reverse-osmosis purified water. pH was approximately 7.4. No further information is available.
Statistical methods:	Not available

Test Conditions: A study was performed to assess the ready biodegradability of the test material in an aerobic aqueous media. The test material was exposed to sewage sludge microorganisms at a concentration of 10 mg C/L with culture medium in sealed culture vessels in the dark at 21°C for 28 days. Following the recommendations of the International Standards Organization, the test material was adsorbed onto granular silica gel prior to dispersion in the test medium in order to aid dispersion of the test material in the test medium and to increase the surface area of the test material exposed to the test organisms. Silica gel was added to the control and standard material vessels in order to maintain consistency between these vessels and the test material vessels. The degradation of the test material was assessed by the determination of carbon dioxide produced. Control solutions with inoculum and the standard material, sodium benzoate, together with a toxicity control, were used for validation purposes.

The validation criteria for this study were:

The standard material yields >=60% degradation by day 14.

The test material may be considered to be readily biodegradable if >=60% degradation is attained after 28 days. This level of degradation must be reached within 10 days of biodegradation exceeding 10%.

The toxicity control should attain >=25% degradation by day 14 for the test material to be considered as non-inhibitory.

The difference of the extremes of replicate values of production of CO2 at the end of the test is less than 20%.

The total CO_2 evolution in the control vessels at the end of the test should not normally exceed 40 mg/L medium.

The Inorganic Carbon content of the test material in the culture media must be less than 5% of the Total Carbon on day 0.

Results

Degradation %:	51% after 28 days
Results:	Not readily biodegradable
Kinetic of Test substance:	1 day = 2% 3 day = 23% 10 day = 35% 16 day = 38% 28 day = 51%
Control substance:	Benzoic acid, sodium salt
Kinetic:	14 day = 71% 28 day = 85%
Breakdown Product:	not measured
Remarks:	The test material attained a total of 51% degradation during the test. The toxicity control attained 51% degradation after 14 days confirming that the test material was not toxic to sewage treatment microorganisms used in the study. C24-30 Alkenes, Branched and Linear cannot be considered to be readily biodegradable under the strict terms and conditions of OECD Guideline No. 301B
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
Reference:	Mead C (2000). C24-30 alkenes, branched and linear: Assessment of ready biodegradability; CO2 evolution test, SafePharm Laboratories Limited, Project No. 703/214. Conducted for Chevron Research and Technology Company (unpublished report).

3.5 BOD5, COD or ratio BOD5/COD

No data available

3.6 Bioaccumulation

Test Substance

Identity: C18-C54 alpha olefins and C18 internal olefin

Method

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.15

Test Conditions: Based on chemical structure and Log Kow (estimated by EPIWIN), using methods of Meylan et al., 1999. The program used the alpha structure for all substances.

Formula used to make BCF estimate for C18: Log BCF = -1.37 log Kow +14.4 + correction (alkyl chains [8+ -CH2- groups] with a value of -1.5).

Formula used to make BCF estimate for C20: Log BCF = -1.37 log Kow +14.4 with no correction.

Formula used to make BCF estimate for C22 – C54: Log BCF = -1.37 log Kow +14.4 with no correction, but a minimum Log BCF of 0.50 was applied.

Results

Value:

Substance	CAS NUMBER	Log Kow used	Estimated Log BCF	Estimated BCF
1-Octadecene	112-88-9	9.04	0.509	3.226
Octadecene	27070-58-2	9.04	0.509	3.226
1-Eicosene	3452-07-1	10.03	0.663	4.603
1-Docosene	1599-67-3	11.01	0.500	3.162
1-Tetracosene	10192-32-2	11.99	0.500	3.162
1-Hexacosene	18835-33-1	12.97	0.500	3.162
1-Octacosene	18835-34-2	13.96	0.500	3.162
1-Triacontene	18435-53-5	14.94	0.500	3.162
C54 Alpha Olefin	--	26.72	0.500	3.162

Reliability: (2) Reliable with restrictions. Value is calculated.

Reference: Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.7 Additional Information

A. **Sewage Treatment**

Test Substance

Identity: C18-C54 alpha olefins and C18 internal olefins

Test Method: Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

Input values: MW; Henry's LC; air-water partition coefficient; Log Kow; biomass to water partition coefficient; temperature = 25°C. A vapor pressure of 6.75 [E-5] mm Hg was used for 1-octadecene. VP was not used for calculations for other substances.

GLP: No

Test Medium: Secondary waste water treatment (water)

Test Type: Aerobic

Test Results:

Substance	MW	Henry's Law Constant (atm-m^3/mol)	Air/Water Partition Coefficient	Log Kow	Biomass/ Water Partition Coefficient	% Removed from Wastewater Treatment
1-Octadecene	252.49	10.7	437.598	9.04	2.19296 [E8]	95
Octadecene	252.49	10.7	437.598	9.04	2.19296 [E8]	95
1-Eicosene	280.54	18.9	772.954	10.03	2.14304 [E9]	94
1-Docosene	308.6	33.4	1365.96	11.01	2.04659 [E10]	94
1-Tetracosene	336.65	58.8	2404.75	11.99	1.95447 [E11]	94
1-Hexacosene	364.7	104	4253.29	12.97	1.86651 [E12]	94
1-Octacosene	392.76	183	7484.16	13.96	1.82402 [E13]	94
1-Triacontene	420.81	322	13168.8	14.94	1.74193 [E14]	94
C54 Alpha Olefin	757.46	289000	1.18192 [E7]	20	2 [E19]	94

Reliability: (2) Reliable with restrictions: Value was calculated.

Reference: EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

4. ENVIRONMENTAL TOXICITY

4.1 Acute Toxicity to Fish

A. Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene (C18 linear alpha olefin)
Remarks:	Source: Shell Chemicals UK Ltd., Stanlow. Stability during use confirmed by infra-red spectra. Density - 0.788 kg/L @ 20°C. Clear, colorless liquid.

Method

Method/guideline:	Similar to OECD 203
Test type:	96-h acute toxicity test (daily static renewal)
GLP:	Yes [X] No [ ]
Year:	1985
Species/Strain:	*Salmo gairdneri*/RT44/Zeals Fish Farm, Wolverton, Wiltshire
Analytical Monitoring:	No
Exposure period:	96 hours
Statistical methods:	Visual inspection

Test Conditions: Fingerlings were obtained from Zeals Fish Farm (UK) and allowed to acclimate to test conditions for more than 10 days prior to exposure. Fish used for testing had an average mean length of 5.4 cm and a mean weight of 2.0 g. Five glass aquariums were obtained and filled with 20 L of filtered (8 μm), dechlorinated laboratory water. Each exposure solution was prepared by adding known quantities of 1-Octadecene to four of the five test aquariums. This resulted in nominal concentrations of 0, 100, 200, 500, and 1000 mg 1-Octadecene/L. The aquarium with no 1-Octadecene served as the untreated control. Ten *S. gairdneri*, previously acclimated to test water, were placed in each test chamber and exposed for 96 hours. Test concentrations were renewed daily. Test waters were gently aerated and organisms were not fed during the 96 hour exposure duration. Water temperatures were maintained between 13.5 and 16.5°C, while pH, hardness and dissolved oxygen ranged from 8.0-8.3 s.u., 220-280 mg/L as $CaCO_3$, and 8.8-10.4 mg/L, respectively.

Results:

Nominal concentrations:	100, 200, 500, 1000 mg/L
Measured concentrations:	Not measured
Element value:	LC0 at 96 hrs> solubility; LL0 = 1000 mg/L (nominal)
Remarks:	The acute toxicity of C18 linear alpha olefin (1-Octadecene) to rainbow trout fingerling, *Salmo gairdneri*, was determined in an acute toxicity test (daily static renewal) with nominal exposures to 100, 200, 500 and 1000 mg 1-Octadecene/L, concentration which are above the water solubility limit. Undissolved test substance was observed at the surface at all concentrations. No mortality was observed at any concentration tested during the 96 h test duration. Therefore, the 96 h LL0 for *S. gairdneri* fingerlings was 1000, the highest concentration tested.

Reliability: (2) Reliable with restrictions. The study was conducted under GLPs and can be considered a guideline study. However, 1-Octadecene was tested at concentrations above the water solubility limit and concentrations were not verified by analysis. Toxicity endpoint was expressed as the initial nominal concentration.

Flag: Key study for SIDS endpoint

References: Pearson N. (1985) C18 Linear Alpha Olefin (1-Octadecene): Acute Toxicity (*Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water coefficient. Shell Research Limited, Sittingbourne Research Center. Shell Report # SBGR.85.059 (unpublished study).

B. Test Substance

Identity: CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

Method

Method/guideline:	OECD 203
Test type:	Semi-static Fish Acute Toxicity Test
GLP:	Yes [X] No [ ]
Year:	1995
Species/Strain:	*Scopthalmus maximus*
Analytical Monitoring:	no
Exposure period:	96 hours
Statistical methods:	Not specified

Test Conditions: Based on range-finding data, the definitive test (semi-static) was conducted on 5 dose levels (loading levels of 1000, 1800, 3200, 5600, and 10000) and a control. Actual concentrations in test media were not measured. Juvenile turbot of approximately 3cm in length were used in all tests. Fish supplied by Mannin Seafarms Ltd. (Scotland) were maintained in controlled conditions of approximately 18 °C with constant illumination. The pH ranged from 7.8 to 8.3. The dissolved oxygen ranged from 85% to 98%. The tests were conducted in 14L capacity moulded soda-lime glass tanks containing 10 liters of test media (1 µm filtered UV treated seawater) . The test material was added directly to the appropriate tank and the test medium was replaced at 48 hours. A single vessel was used per test concentration and gentle aeration was supplied. Ten animals were exposed per test concentration for 96 hours with observations being conducted at 24 hour intervals.

Results: After 96 hours, no mortality was observed at the maximum dose level of 10,000 mg/L (loading levels), therefore, the LC50 was greater than solubility; the LL0 was10,000 mg/L.

Reliability: (2) Reliable with restrictions. The study was conducted under GLPs and can be considered a guideline study. However, the test substance was tested at concentrations above the water solubility limit and concentrations were not verified by analysis. Toxicity endpoint was expressed as the initial nominal concentration. Also, constant illumination was used during the study instead of the recommended 12-16 hour photoperiod.

References: Environment & Resource Technology Ltd. (1997) Assessment of the aquatic-phase toxicity of C16-C18 Alpha Olefin Isomerized Base Fluid to the marine fish, *Scopthalmus maximus*, Study No. 074-5-1. Conducted for Chevron Chemical Company (unpublished report).

C. Test Substance

Identity: CAS No. 93924-10-8, C20-24 Alpha Olefin

Remarks: Composition: <47% C20, <35% C22, <26% C24, <3% C18, <1% C16; 89.3% linear, 8.3% branched

Method

Method/guideline:	OECD 203
Test type:	96 hour semistatic toxicity test
GLP:	Yes
Year:	1993
Species/Strain:	Rainbow trout *(Oncorhynchus mykiss)*
Analytical Monitoring:	Yes
Exposure period:	96 hr
Statistical methods:	As there were no mortalities, statistical methods were not warranted

Test Conditions: The water accommodated fraction (WAF) was prepared by mixing 1000 mg/l of GULFTENE 20-24 with water. The mixture was stirred on magnetic stirrers for 24 hours at 14°C and then allowed to settle for approximately 1 hour. The WAF was then withdrawn via a siphon prior to dilution to the required exposure levels and testing.

Water samples were taken from the control and each exposure level at 0 hours for test concentration verification. The concentrations were analyzed using an Ionics TC/TOC Analyser Model 555. Since the values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than the control level, analysis was not carried out at other time points.

Juvenile fish were obtained from Westacre Trout Farm, Norfolk, U.K. The mean standard length, determined by measuring the control fish at the end of the exposure period, was 5.1 cm (SD = 0.5 cm) and the mean weight was 1.73 g (SD = 0.51 g). Groups of ten fish (5 test concentrations plus one control) were exposed for 96 hours to dilution

series of a single WAF of GULFTENE 20-24 (100 % WAF equivalent to 1000 mg/L). Animals were placed at random in glass aquaria containing prepared test media or diluent water only. Each vessel contained 20 L of medium to a depth of 19 cm (approx. dimensions of vessel: 25x46x25 cm). This provided an initial loading of 0.87 g b.w./L (static volume). Supplementary aeration was provided. Temperature was maintained at 13-14°C. Photoperiod: 16 hr light: 8 hr dark. Fish were not fed during the exposure period. pH ranged from 7.6 to 8.2. Dissolved oxygen ranged from 9.9 to 10.2 mg O_2/L. The test concentrations were 10, 18, 32, 56, and 100% WAF. Observations were made on the numbers of dead fish and the incidence of sub-lethal effects after 3, 6, 24, 72 and 96 hours exposure.

Results: LC_{50} (96 hr) > solubility
LL0 = 1000 mg/L loading rate WAF

Remarks: There were no mortalities observed during the study. Slight loss of equilibrium and lethargy were observed at the 100% WAF (1000 mg/L) only.

TOC analysis values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than those for the control level. Thus, actual concentrations were negligible.

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint

References: Huntingdon Research Centre (1993) Gulftene 20-24 (water accommodated fraction) acute toxicity to rainbow trout, Project CHR 46(D)/930361. Conducted for Chevron Research and Technology Company (unpublished report).

D. Test Substance

Identity: CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline: OECD 203
Test type: 96 hour semi-static toxicity test
GLP: Yes
Year: 1998
Species/Strain: Rainbow trout *(Oncorhynchus mykiss)*
Analytical Monitoring: Yes
Exposure period: 96 hr

Statistical methods: Moving average method of Thompson (1947)

Test Conditions: A study was performed to assess the acute toxicity of the test material, C20-24 Alkenes, Branched and Linear, to rainbow trout. Following a preliminary range-finding study, fish were exposed, in three groups of ten, to a Water Accommodated Fraction (WAF) of the test material for a period of 96 hours. A semi-static test regime was employed in the study involving a daily renewal of the test preparations to ensure that the concentrations of the test material remained near nominal and to prevent the build up of nitrogenous waste products. The WAF was prepared by placing the test material on the surface of water to give a 1000 mg/L loading rate which was then stirred with a magnetic stirrer to achieve a vortex depth of approximately 5% of the distance to the bottom of the vessel, for 24 hours. The mixture was then allowed to stand for 4 hours prior to removing the aqueous phase or WAF by siphon. Test vessels were 20 L glass aquaria containing 20 L of test solution. Each vessel was covered to reduce evaporation after 10 fish were added and maintained at 14°C in a temperature-controlled room with a 16-hour light and 8-hour dark cycle. Dissolved oxygen ranged from 9.4 to 9.7 mg/L for fresh solutions and 8.6 to 8.8 for old solutions. The pH ranged from 7.4 to 7.5 for fresh solutions and 7.2 to 7.4 for old solutions. The vessels received no auxiliary aeration.

Analysis of the WAF was carried out by Total Organic Carbon (TOC) analysis on samples from each of two replicate vessels of the treated and the control media at the beginning and end of the first 24 hours of the test.

Dilution water chemistry: approximately 100 mg/L (as CaCO3) total hardness; 1.5 mg C/L total organic carbon content; 0.20 mg/L particulate matter; pH 7.6; $\geq$ 9.2 mg/L dissolved oxygen.

Fish supplied by Brow Well Fisheries Ltd, Phoenix Cottage, Hebden, Nr. Skipton, UK, were juvenile ($\leq$ 3 months). A mean weight and length were 0.88 g and 4.2 cm, respectively at the end of the study. Based on the mean weight value, loading rate was 0.44 g bodyweight/L.

The number of mortalities and any adverse reactions to exposure in each test and control vessel were determined 3 and 6 hours after the start of exposure and then daily throughout the study until termination after 96 hours. Duplicate control groups were maintained under identical conditions but not exposed to the test material.

Results:

LC50: > solubility at 96 hrs; LL0 = 1000 mg/L loading rate WAF at 96 hrs

Remarks: In the Range-finding study the results showed no mortalities at the 10, 100, and 1000 mg/L loading rate WAF's.

The results of the definitive study showed that the highest loading rate WAF (1000 mg/L) produced 0% mortality and no adverse effects.

The results of the TOC analysis showed that, compared to the controls, no significant levels of carbon were detected in the WAFs. Thus, actual concentrations were negligible.

The 96-hour median Lethal Loading Rate (LLR50) for the test material to rainbow trout (Oncorhynchus mykiss), based on nominal loading rates, was greater than 1000 mg/L loading rate WAF and, correspondingly, the No Observed Effect Concentration was greater than solubility. The LL0 was 1000 mg/L loading rate WAF.

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint

References: Handley JW, Sewell IG, and Bartlett AJ (1998) C20-24 Alkenes, Branched and Linear: Acute Toxicity To Rainbow Trout, Project No.703/123. Conducted for Chevron Research and Technology Company (unpublished report).

4.2 Acute Toxicity to Aquatic Invertebrates (e.g. Daphnia)

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene; C18 linear alpha olefin

Remarks: Source: Shell Chemicals UK Ltd., Stanlow. Stability during use confirmed by infra-red spectra. Density - 0.788 kg/L @ 20°C. Clear, colorless liquid.

Method

Method/guideline:	Similar to OECD 202
Test type:	48-h acute toxicity test (static)
GLP:	Yes
Year:	1985
Analytical Monitoring:	No
Species/Strain:	*Daphnia magna*
Supplier:	Strain obtained from I.R.Ch.A., France
Exposure period:	48 hrs
Statistical methods:	Visual inspection

Test Conditions: Quantities of 1-Octadecene were added to 140-mL flasks so that, when brought to 140 ml final volume with a reconstituted freshwater, nominal concentrations equaled 100, 200, 500 and 1000 mg 1-Octadecene/L. Flasks were prepared in triplicate and three flasks served as untreated laboratory controls. Ten *Daphnia magna* (less than 24 h old) were placed in each test flask. To minimize the risk of these organisms

becoming trapped at the surface, black plastic caps were placed just beneath the water surface to create a darkened zone that *D. magna* would avoid. The numbers of immobilized *D. magna* were recorded after 24 and 48 hours. Test temperatures ranged between 18-22°C, pH ranged from 7.8 to 8.0 s.u. and dissolved oxygen concentrations ranged between 8.6 and 9.0 mg/L. The total hardness of the reconstituted laboratory water was 170 mg/L as $CaCO_3$.

Results:

Nominal Concentrations:	100, 200, 500, and 1000 mg/L
Measured Concentrations:	Not measured
Element value:	EC50 at 48 hrs > solubility; the EL50 was >1000 mg/L (nominal)
Remarks:	Concentrations of 100, 200, 500, and 1000 mg 1-Octadecene/L were not completely soluble and were visible at the surface as floating globules. The acute toxicity of C18 linear alpha olefin to the crustacean zooplankter, *Daphnia magna*, was determined in a static acute toxicity test with nominal concentrations which were above the water solubility limit. Undissolved test substance was observed at the surface at all concentrations. Less than 4% of *D. magna* were immobilized during 48 h exposure to 1000 mg/L of the olefin, the highest nominal concentration tested. The 24 and 48 h EL50 values were therefore both greater than 1000 mg/L.
Reliability:	(2) Reliable with restrictions. The study was conducted under GLPs and can be considered a guideline study. However, 1-octadecene was tested at concentrations above the water solubility limit and concentrations were not verified by analysis. Toxicity endpoint was expressed as the initial nominal concentration.
Flag:	Key study for SIDS endpoint
References:	Pearson N. (1985). C18 Linear Alpha Olefin (1-Octadecene): Acute Toxicity (*Salmo gairdneri, Daphnia magna and Selenastrum capricornutum*) and n-octanol/water coefficient. Shell Research Limited, Sittingbourne Research Center. Shell Report # SBGR.85.059.

B. Test Substance

Identity:	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 202
Test type:	48-h aqueous toxicity test (static)
GLP:	Yes
Year:	1998
Analytical Monitoring:	Yes
Species/Strain:	*Daphnia magna*
Supplier:	Strain obtained from I.R.Ch.A., France
Exposure period:	48 hrs
Statistical methods:	No specifics noted

Test Conditions:

A study was performed to assess the acute toxicity of the test material, C20-24 Alkenes, Branched and Linear, to *Daphnia magna*. Following a preliminary range-finding study, forty daphnids (4 replicates of 10 animals) were exposed to a Water Accommodated Fraction (WAF) of the test material for 48 hours under static test conditions. The WAF was prepared by placing the test material on the surface of the water to give a 1000 mg/L loading rate which was then stirred by magnetic stirrer to achieve a vortex depth of approximately 5% of the distance to the bottom of the vessel for 24 hours. The mixture was then allowed to stand for 4 hours prior to removing the aqueous phase or WAF by siphon. Test vessels were 250 mL glass jars containing approximately 200 mL of test solution. Each vessel was covered to reduce evaporation and maintained at 21°C in a temperature-controlled room with a 16-hour light and 8-hour dark cycle. Dissolved oxygen was from 8.2 to 8.4 mg/L for fresh solutions and 8.1 for old solutions. The pH was 7.9 for fresh and old solutions. The vessels received no auxiliary aeration.

Analysis of the WAF was carried out by Total Organic Carbon (TOC) analysis on the test preparation at 0 and 48 hours.

Daphnia magna were supplied by the Institute National de Recherché Chimique Appliquée, France. Adult daphnia were maintained in polypropylene vessels and each culture was fed daily with a suspension of mixed algae. Culture conditions ensured that reproduction was by parthenogenesis. Gravid adults were isolated 24 hours prior to the initiation of the study, the young daphnids produced overnight were then removed for testing.

Immobilization and any adverse reactions to exposure were recorded after 24 and 48 hours. Replicate control groups were maintained under identical conditions but not exposed to the test material.

Results

Element value:	48 hr EC50 > solubility; EL0 = 1000 mg/L loading rate WAF at 48 hrs
Remarks:	In the Range-finding study the results showed no immobilization at the 10, 100, and 1000 mg/L loading rate WAF.
	In the Definitive study, there was no immobilization in 40 daphnids exposed to a 1000 mg/L loading rate WAF for a period of 48 hours.

Therefore, the 48-hour median Effective Loading Rate (ELR50) for the test material to *Daphnia magna*, based on nominal loading rates, was greater than 1000 mg/L loading rate WAF; and, correspondingly, the No Observed Effect Concentration, based upon zero immobilization at this concentration, was greater than or equal to 1000 mg/L loading rate WAF.

The results of the TOC analysis showed that compared to the controls, no significant levels of carbon were detected in the WAFs. Thus, actual concentrations were negligible.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Handley JW, Wetton PM, and Bartlett AJ (1998) C20-24 Alkenes, Branched and Linear: Acute Toxicity To Daphnia Magna, Project No. 703/124. Conducted for Chevron Research and Technology Company (unpublished report).

4.3 Toxicity to Aquatic Plants (e.g. Algae)

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene; C18 linear alpha olefin

Remarks: Source: Shell Chemicals UK Ltd., Stanlow. Stability during use confirmed by infra-red spectra. Density - 0.788 kg/L @ 20°C. Clear, colorless liquid.

Method

Method/guideline:	Similar to OECD 201
Test type:	4-day growth inhibition test (static)
GLP:	Yes [X] No [ ]
Year:	1985
Analytical Monitoring:	No
Species/Strain:	*Selenastrum capricornutum*
Source:	ATCC 22662/American Type Culture Collection, Maryland, USA.
Element basis:	500 cells/ml
Exposure period:	72 hrs
Statistical methods:	Visual inspection

Test Conditions: *S. capricornutum* were obtained from the axenic laboratory culture derived from a strain obtained from the American Type Culture Collection (Maryland, USA). Sixteen Erlenmeyer flasks containing 50 ml of culture medium were prepared. Quantities of 1-Octadecene in Analar Acetone were added to ten vessels to obtain nominal concentrations of 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000 mg 1-Octadecene/L. The remaining six flasks received no 1-Octadecene,

however, acetone concentrations in all flasks (including the controls) were adjusted to 0.1 mg/L.

Each flask was inoculated with *S. capricornutum* to an initial concentration of 500 cells/mL. Flasks were incubated at 100 cycles/min under constant illumination (approximately 3000 lux). Tests temperatures ranged from 22-26°C and pH of test solutions ranged from 7.4-7.7 s.u.

Results:

Nominal Concentrations: 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460 and 1000 mg/L

Measured Concentrations: Not measured

Element value: EC50 at 96 hrs > solubility; EL0 = 1000 mg/L, NOEC = 1000 mg/L (nominal)

Remarks: The acute toxicity of C18 Linear Alpha Olefin to the planktonic algae, *Selenastrum capricornutum*, was determined in a 4 day growth test with nominal concentrations that were above the water solubility limit. Undissolved test substance was observed at the surface at 10 mg/L and above. None of the concentrations of the olefin tested caused a reduction in cell number at day 4 compared to the mean cell number at day 4 in the controls. The96 h NOEC was therefore 1000 mg/L (nominal) and the 96 h EL0 was therefore 1000 mg/L, the highest concentration tested.

Reliability: (2) Reliable with restrictions. The study was conducted under GLPs and can be considered a guideline study. However, 1-octadecene was tested at concentrations above the water solubility limit, and concentrations were not verified by analysis. Toxicity endpoint was expressed as the initial nominal concentration.

Flag: Key study for SIDS endpoint

References: Pearson N. (1985) C18 Linear Alpha Olefin (1-octadecene): Acute Toxicity (*Salmo gairdneri, Daphnia magna and Selenastrum capricornutum*) and n-octanol/water coefficient. Shell Research Limited, Sittingbourne Research Center. Shell Report # SBGR.85.059 (unpublished report).

B. Test Substance

Identity: CAS No. 93924-10-8, C20-24 Alpha Olefin

Remarks: Composition: <47% C20, <35% C22, <26% C24, <3% C18, <1% C16; 89.3% linear, 8.3% branched

Method

Method/guideline:	OECD 201
Test type:	static
GLP:	Yes [X] No [ ]
Year:	1993
Analytical Monitoring:	Yes
Species/Strain:	*Selenastrum capricornutum*
Element basis:	Growth rate, area under curve
Exposure period:	72 hrs
Statistical methods:	Not specified

Test Conditions:

Algae were originally obtained from the Culture Centre of Algae & Protozoa c/o Freshwater Biological Association, Cumbria, U.K. Sterile nutrient medium (as recommended in OECD Guideline 201) was inoculated from a master culture and incubated under continuous illumination (~7000 lux) and stirring (orbital shaker) at 24°C to give an algal suspension in log phase growth characterized by an absorbance of 0.870 @ 665 nm.

The water accommodated fraction (WAF) was prepared by mixing 1000 mg/l GULFTENE 20-24 with water. The mixture was stirred on a magnetic stirrer for 24 hours at 24°C and then allowed to settle for approximately 1 hour. The WAF was then withdrawn via a siphon and 100ml was measured into 250ml conical flasks. Flasks were prepared and 2ml of a concentrated algal suspension of *Selenastrum capricornutum*, (0.870 absorbance @ 665 nm) were added to each flask in order to produce the correct starting cell density. Algal cultures were exposed to 6 replicates of a single WAF of GULFTENE 20-24 (100% WAF equivalent to 1000 mg/L). Flasks were loosely stoppered. The exposed cultures plus one control (6 replicates) were incubated without media renewal on an orbital shaker (120 cycles/min) under continuous illumination (~7000 lux) at 24°C for 72 hours. Growth was monitored daily by measuring the absorbance of each culture at 665 nm. The cell densities at initiation and termination for the control were determined by direct counting with a haemocytometer.

Water samples were taken from the control and each exposure level at 0 hours for test concentration verification. The concentrations were analyzed using an Ionics TC/TOC Analyser Model 555. Since the values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than the control level, analysis was not carried out at other time points.

Results:

Element value:	E_bC50 > solubility at 72 hrs
	E_rC50 > solubility at 72 hrs
	NOEC = 1000 mg/L loading rate WAF at 72 hrs
	EL0 = 1000 mg/L loading rate WAF at 72 hrs

Remarks:	The mean cell density of the control at 0 hours was 8.25 x 10[4] cells/ml and at 72 hours was 2.78 x 10[6] cells/ml. All test and control cultures were inspected microscopically at 72 hours. There were no abnormalities detected. The TOC values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than those of the control level; thus, the actual concentrations were negligible.
Reliability:	(1) Reliable without restrictions.
Flag:	Key study for SIDS endpoint
References:	Huntingdon Research Centre (1993) Gulftene 20-24 (water accommodated fraction) Algal Growth Inhibition, Project No. CHR 46(A)/930362. Conducted for Chevron Research and Technology Company (unpublished report).

C. Test Substance

Identity:	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 201
Test type:	static
GLP:	Yes [X] No [ ]
Year:	1998
Analytical Monitoring:	Yes
Species/Strain:	Algae (*Pseudokirchneriella subcapitata*, formerly known as *Selenastrum capricornutum*)
Element basis:	Growth rate
Exposure period:	96 hrs
Statistical methods:	Student's t-test

Test Conditions:

A study was performed to assess the effect of the test material, C20-24 Alkenes, Branched and Linear, on the growth of Pseudokirchneriella subcapitata (formerly Selenastrum capricornutum). Following a preliminary range-finding study, Pseudokirchneriella subcapitata was exposed to a Water Accommodated Fraction (WAF) of the test material (six replicate flasks) for 96 hours under constant illumination (intensity approximately 7000 Lux) and shaking at a temperature of 24°C.

The WAF was prepared by dispersing the test material onto the surface of 2 L of culture medium to give a 2000 mg/L loading rate which was then stirred to achieve a vortex depth of approximately 5% of the distance to the bottom of the vessel for 24 hours. The mixture was then allowed to stand for 4 hours prior to removing the aqueous phase or WAF by siphon. An aliquot (500 mL) of the WAF was mixed with algal

suspension (500 mL) to give the test concentration of 1000 mg/L loading rate WAF. Test vessels were 250 mL glass conical flasks containing approximately 100 mL of test solution, covered with aluminum foil to reduce evaporation. Analysis of the WAF was carried out by Total Organic Carbon (TOC) analysis on samples from two replicate vessels of treated and control media at the beginning and end of the test.

Liquid cultures of Pseudokirchneriella subcapitata were obtained from the Culture Centre for Algae and Protozoa (CCAP), Institute of Freshwater Ecology, Ferry House, Ambleside, Cumbria. At initiation of the study the culture contained a nominal cell density of 10000 cells per mL.

Samples of the algal populations were removed daily, and algal cell concentrations were determined, using an electronic cell counter, for each control and treatment group. Triplicate control groups were maintained under identical conditions but not exposed to the test material.

A Student's t-test was carried out on the area under the growth curve data at 96 hours for the control and 1000 mg/L loading rate WAF test concentration to determine any statistically significant differences between the test and control groups.

Results

Element value: EC50 at 96 hrs > solubility; EL0 = 1000 mg/L loading rate WAF

NOEC at 96 hrs = 1000 mg/L loading rate WAF

Remarks: In the Range-finding study the results showed no effect on growth at either concentration, 100 or 1000 mg/L WAF.

From the results of the definitive study neither the growth or the biomass of Pseudokirchneriella subcapitata (formerly Selenastrum capricornutum) were affected by the presence of the test material over the 96-hour exposure period.

All test and control cultures were inspected microscopically at 96 hours. There were no abnormalities detected in any of the control or test cultures.

Exposure of Pseudokirchneriella subcapitata (formerly Selenastrum capricornutum) to the test material gave median Effective Loading Rate zero (EL0) values of 1000 mg/L loading rate WAF and, correspondingly, the No Observed Effect Concentration was 1000 mg/L loading rate WAF.
The results of the TOC analysis showed that, compared to the controls, no significant levels of carbon were detected in the WAFs. Thus, the actual concentrations were negligible

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint

References: Handley JW, Mead C, and Bartlett AJ (1998) C20-24 Alkenes, Branched and Linear: Algal Inhibition Test, Project No. 703/125. Conducted for Chevron Research and Technology Company (unpublished report).

4.4 Toxicity to Micro-organisms, e.g. Bacteria

A. Test Substance

Identity: CAS No. 112-88-9, 1-Octadecene

Method

Method: 79/931/EEC, Annex V, According *to Degradability, Ecotoxicity, and Bioaccumulation*, TNO, Delft, The Netherlands, 1977

GLP: No

Species: *Pseudomonas fluorescens*

Exposure Period: 6 hours

Analytical Monitoring: No data

Test Conditions: The test material was dissolved in ethanol to give a stock solution containing 500 g/l of 1-octadecene. Dilutions of the stock solution in test medium were made such that the final concentrations were 1000, 320, 100, 32 and 10 mg/l. Sodium pentachlorophenate was used as a standard inhibitory substance. Controls containing the microbial inoculum and no inhibitory substances were used to assess the logarithmic growth rate of the organisms under non-inhibitory conditions. Growth curves were constructed of the optical density of the inoculated media versus time and the rate determined as the slope of the exponential growth phase.

$$\% \text{ inhibition} = \frac{\text{growth rate control- growth rate test}}{\text{growth rate control}} \times 100$$

Results: EC50 >1000 mg/L

Remarks: The standard substance, sodium pentachlorophenate inhibited with an EC50=31.5 mg/l while the test substance caused no significant inhibition at concentrations up to 1000 mg/l.

Reliability: (1) Reliable without restriction

Reference: Watkinson, R.J. (1985) C18 Linear Alpha Olefin: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center. Shell Report # SBGR.85.115 (unpublished report).

B. Test Substance

Identity: CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method:	OECD 209
GLP:	Yes
Type:	Aquatic, aerobic
Year:	1997
Species:	Sewage sludge micro-organisms
Exposure Period:	3 hours
Analytical Monitoring:	No

Test Conditions: A study was performed to assess the effect of the test material on the respiratory rate of sewage sludge micro-organisms under aerobic conditions. The activated sewage sludge sample was maintained on continuous aeration at 21°C and used on the day of collection. The pH was 7.6 and suspended solids equal to 3.6 g/L. Test water was dechlorinated laboratory tap water with total hardness of ~ 100 mg/L as $CaCO_3$. Synthetic sewage (g/L water): 16 peptone, 11 meat extract, 3 urea, 0.7 g NaCl, 0.4 $CaCl_2.2H_20$, 0.2 $MgSo_4.7H_2O$, 2.8 K_2HPO_4.

A rangefinding study was conducted with concentrations of 100 and 1000 mg/L. For the definitive study, test material (500 mg) was dispersed in ~ 250 ml water in a conical flask and ultrasonicated for ~ 30 min. Synthetic sewage (16 ml), activated sewage sludge (200 ml, predominantly domestic sewage) and water were added to a final volume of 500 ml to give a concentration of 1000 mg/L. The mixture was aerated with compressed air via narrow bore glass tubes at a rate of ~ 0.5-1 L/min. The study with 3 replicates was conducted at 21°C under normal laboratory lighting for 3 hours. Duplicate controls consisted of inoculum exposed to the synthetic sewage sludge and water. Control solutions with inoculum and the standard material (3,5-dichlorophenol, 3.2, 10 and 32 mg/L) were used for validation purposes.

Respiration rates were determined by measuring oxygen consumption at 30 minutes and 3 hours. An aliquot was poured into a BOD bottle and the rate of respiration measured using a Yellow Springs dissolved oxygen meter fitted with a BOD probe. The rate of respiration for each flask was measured over the linear portion of the oxygen consumption trace for an approx. 10 min period (between ~ 8.5 mg O_2/L and 1.4 mg O_2/L).

To calculate the inhibitory effect of the test and reference materials, the respiration rate was expressed as a percentage of the 2 control respiration rates. Percentage inhibition was plotted against concentration and the EC_{50} values derived by inspection of the graph. The results of the study were considered valid if (1) the 2 control respiration rates were within 15% of each other and (2) the EC_{50} (3-hr contact time) for 3.5-dichlorophenol lay within the range 5-30 mg/L.

Results:

EC_{50} of test material:	>1000 mg/L at 30 min and 3 hr
EC_{50} of standard:	16 mg/L at 30 min and 11 mg/L at 3 hr
NOEC of test material:	≥1000 mg/L

Remarks: Under the conditions of the test, the test material did not inhibit the respiration rate of activated sewage sludge. The validation criteria were satisfied.

Reliability: (1) Reliable without restrictions

Reference: Mead, C. (1998) C20-24 Alkenes, Branched and Linear: Activated Sludge Respiration Inhibition OECD 209. Conducted by Safepharm Laboratories, Ltd., Project No. 703/126. Report to Chevron Research and Technology Company (unpublished report).

4.5 Chronic Toxicity to Aquatic Organisms

No data available

4.6 Toxicity to Terrestrial Organisms

A. Toxicity to Terrestrial Plants.

No data available

B. Toxicity to Soil Dwelling Organisms.

No data available

C. Toxicity to Other Non Mammalian Terrestrial Species (including Avian)

No data available

4.7 Biological EffectsMonitoring (including Biomagnification)

No data available

4.8 Biotransformation and Kinetics

No data available

4.9 Additional Information

No data available

5. MAMMALIAN TOXICITY

5.1 Toxicokinetics, Metabolism and Distribution

A.	**Test Substance:**	CAS No. 112-88-9 (1-octadecene), cis- and trans-9-nonadecene, n-paraffins C14-C30, 8-hexadecyne, pentadecylcyclohexane
	Method	Non-standard
	Test Type	in-vivo
	GLP	No data
	Year	No data
	Method:	Mixtures of hydrocarbons, always including squalane, were prepared involving 3 or 4 different hydrocarbons in an equal weights ratio and administered to rats. Feces was analyzed to determine the percentage retained in the animal. Preliminary experiments revealed that 96-100% of squalane fed to rats could be recovered in feces collected for 4 days following administration. This was the case whether fed or fasted rats were used, and whether the squalane was administered by stomach tube in bulk or as a solution in corn oil, or fed as a mixture with the standard diet wafers. Holding the feces at room temperature or at 37 ° C for up to 72 h after collection did not reduce the recovery of squalane, indicating the absence of bacterial attack. No squalane was detected in the 72-h urine of 400 g rats given 85-mg doses of squalane by stomach tube. Bile collected for 8 h and lymph collected for 5 h after administration of squalane did not contain detectable amounts of the hydrocarbon (*i.e.* less than 0.01 μg/ml). 72 h after the administration of squalane only 120 ± 10 μg of hydrocarbon, 0.14 % of the dose, could be recovered from extracts of the entire gastrointestinal tract including its contents. Finally, when a mixture of squalane-n-octadecane -n-octacosane (1:1:1, by weight) was administered to a rat, the ratio of components in the feces was constant over a 72-h period. These observations supported the use of squalane as an oilphase marker for the balance study.

Test Conditions: Mixtures were administered at various dose levels (0.8 ml/kg bw) to fed, 250 g rats by stomach tube. Rats were allowed food and water *ad libitum* while feces were collected twice daily and stored in chloroform until excretion of the hydrocarbon ceased (72-96 h). Both test feces and control feces to which had been added aliquots of the hydrocarbon mixture being tested were extracted and the hydrocarbons were analyzed by gas chromatography (HP Model 5750 and Varian Aerograph Model 1200 gas chromatographs equipped with hydrogen flame ionization detectors). The percentage of each hydrocarbon "retained" by the animals was considered to be 100% minus the percentage excreted, and was calculated from the formula $R = [(A/S)_D - (A/S)_F)/(A/S)_D] \times 100\%$, where R = percentage retained, A/S = molar ratio of test hydrocarbon to squalane, D refers to the diet and F to the feces. Each hydrocarbon was tested in three animals and each feces sample was analyzed at least 3 times.

Species: Rat

Strain: CD

Sex: Male

Age: No data

Bodyweight: 250 g

Number of Animals: 3 per hydrocarbon

Route: oral gavage

Dose(s) used: 60 – 530 mg/kg bodyweight (tested hydrocarbons), 50-500 mg/kg (squalane)

Statistical Methods: Linear regression, 2-tailed t-test

Results: The percentage retention of n-alkanes showed an inverse linear relationship to chain length that was describable by the regression line: (percentage retained) = 115. 9 - 3.94 x (number of carbon atoms). This line had a correlation coefficient of - 0.995, standard error of estimate Sy- x = 3.30, t = 30.85 and P< 0.001 (Croxton, 1953). Paraffins having more than 29 carbon atoms thus would not be absorbed to a significant extent under these conditions. The branched, cyclic and unsaturated hydrocarbons examined in this study, when compared to the corresponding n-saturated hydrocarbons of the same total number of carbon atoms, all gave P>0. 9 (2-tailed t-test) or no statistically significant difference in percentage retention. Thus carbon number appeared to be the determining factor in retention under these conditions. The effect of dose on percentage retention was similar for all of those hydrocarbons retained to a sufficient extent to permit detection of small differences, The percentage retained was constant between 60 and approx. 320 mg/kg rat, but fell off above this level. The retention was

only 70 % of maximum at a dose of 530 mg/kg rat. The relative amount of squalane (50 – 500 mg/kg bw) in the mixture had no detectable effect on the retention of the other components.

Reliability: (1) Reliable without restrictions.

Reference: Albro PW and L Fishbein. (1970) Absorption of aliphatic hydrocarbons by rats. Biochim. Biophys. Acta 219:437-446.

Croxton, F.E. (1953) Elementary Statistics with Applications in Medicine and the Biological Sciences, Dover Publications, Inc. New York.

B. Test Substance: Mineral oils and waxes

Method	Non-standard
Test Type	in-vivo
GLP	No data
Year	No data

Method: Determination of the molecular weight distribution of hydrocarbons extracted from female rat livers from two 90-day feeding studies conducted at BIBRA Toxicology International (CONCAWE, 1993)with a variety of oils and waxes, and from the original test samples. Also, an analysis was carried out on the livers of rats that were subjected to a 28 day recovery period (first study) and a 90 day recovery period (second study).

Test Conditions: First study: Tissues were homogenized in 70% KOH using an Ultraturrax blade homogenizer. Approximately 1 g tissue was cut from the periphery of the liver, homogenized and used for the tissue analysis. If repeat analysis was necessary, a further portion was cut away, homogenized and analyzed. Samples supplied for GLC analysis were prepared from tissue remaining after storage at -10°C since necropsy. Homogenates or aliquots of homogenate were extracted into 20 ml carbontetrachloride at 60°C in an ultrasonic bath for 30 minutes. After centrifugation, 8 ml aliquots were passed through columns of partially deactivated Florisil, collecting to a final volume of 10 ml. This extract was then analyzed by FTIR for mineral hydrocarbon content. The extracts were than evaporated to dryness under nitrogen in the containers for transport.

Second study: The entire liver sample was homogenized in 70% KOH using an Ultraturrax blade homogenizer, using 3 ml KOH for each whole gram of tissue. The volume of the homogenate was measured and a 3 ml aliquot taken for extraction, column clean-up, analysis and to provide the samples for GLC analysis. The homogenates or aliquots of homogenate were extracted into 20 ml carbontetrachloride at 60°C in an ultrasonic bath for 30 minutes. After centriguation, 8 ml aliquots were passed through columns of partially deactivated Florisil, collecting to a final

volume of 10 ml. This extract was then analyzed by FTIR for mineral hydrocarbon content.

Female rats received either control diet or 2% w/w test article in diet for 90 days. Reversal group received control diet for the reversal period. Samples for analysis were stored at -20°C. For chromatographic analysis, the residues were dissolved in iso-octane p.a.

Conversion of chromatograms: In the case of oils, raw GC data were converted to boiling point distributions (BPD) using ASTM D-2887. The waxes were analyzed following the EWF-method (determination of n- and iso-paraffins content and their carbon number spread by cold-on-column capillary GC method). In this method, the total carbon distribution of the wax is expressed as normal- and isopercentage (iso has to be read as non-normal, mainly branched paraffins). For comparison's sake the carbon number distribution of the waxes was in some cases converted to BPD, using the (expanded) ASTM D-2887 conversion table.

Species:	Rat
Strain:	F344
Sex:	Female
Number of Animals:	Liver tissue from single animals (Study 1) and single samples of pooled liver extracts of 5 animals (Study 2)
Route:	Feeding study – in diet
Dose(s) used:	Study 1: 0, 0.002, 0.02, 0.2 and 2.0 % in diet Study 2: 0, 0.02, 0.2 and 2.0 % in diet
Results:	Lower and/or higher molecular weight fractions were underrepresented in the liver extracts, and no hydrocarbons with carbon numbers over C35 (boiling point 491°C) were found. In liver extracts from the 28-day reversal group, a substantial reduction in quantity of the deposited hydrocarbons was observed. After the 90-day reversal period, the deposits were further decreased.
Reliability:	(1) Reliable without restrictions.
Reference:	de Rooij JF, Woldhuis J, Kemp G, Kollard H (1993) Analysis of hydrocarbon residues in rat livers. Appendix to CONCAWE Report No. 93/56. CONCAWE, Brussels.

5.2 Acute Toxicity

A. Acute oral toxicity

(1) **Test Substance**

Identity (purity): C14-18 Alpha Olefin

Remarks: Blend of CAS No. 1120-36-1, 1-Tetradecene; CAS No. 629-73-2, 1-Hexadecene; CAS No. 112-88-9, 1-Octadecene (proportions unknown)

Method

Method/guideline: 16 CFR 1500.3 (c)(2)(i)
Type *(test type):* LD50
GLP: No
Year: 1977
Species/Strain: Rat/CFE
Sex: Male and female
No. of animals per sex per dose: 5

Vehicle: None specified
Route of administration: Oral gavage

Test Conditions: Ten healthy CFE rats (5M:5F) with body weights averaging approximately 250 grams were used to determine the oral toxicity of the test sample. Animals were fasted approximately 18 hours prior to dosing but had ready access to water. Each rat received a single oral dose of 10 grams/kg body weight of test compound by gastric intubation. Animals were observed for mortality and body weight changes for 14 days post-dosing. All surviving animals were sacrificed and necropsies were performed.

Results:

Value: LD50 > 10 g/kg
Number of deaths at each dose level: No deaths were observed

Remarks:

Sex	Initial Body Weight	Final Body Weight
M	277	320
M	262	319
M	272	334
M	273	346
M	262	317
F	230	264
F	228	248
F	227	262
F	217	276

F	236	268

All rats dosed with 10 grams/kg body weight survived the 14-day observation period. No signs of intoxication were seen during the observation period. The oral LD50 for the test material was determined to be greater than 10 grams/kg body weight. Body weight gain was within normal limits.

Gross autopsy findings revealed blanched and mottled kidneys in most rats.

Under the conditions of the test, the study material is not considered to be a toxic substance when administered by the oral route.

Reliability: (2) Reliable with restrictions Age of animals and analytical composition was not reported

Flag: Key study for SIDS endpoint.

References: Ethyl (1977) Toxicology Evaluation of Ethyl Compound 100-606. Gulf South Research Institute P.O. Box 1177 New Iberia, LA 70560 (unpublished report).

(2) Test Substance

Identity (purity): C18-C24 Alpha Olefin

Remarks: Blend of CAS No. 112-88-9, 1-Octadecene; CAS No. 3452-07-1, 1-Eicosene; CAS No. 1599-67-3, 1-Docosene; CAS No. 10192-32-2, 1-Tetracosene (proportions unknown)

Method

Method/guideline:	16 CFR 1500.3 (c)(2)(i)
Type *(test type):*	LD50
GLP:	No
Year:	1977
Species/Strain:	Rat/CFE
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	None specified
Route of administration:	Oral gavage

Test Conditions: Ten healthy CFE rats (5M:5F) with body weights averaging approximately 250 grams were used to determine the oral toxicity of the test sample. Animals were fasted approximately 18 hours prior to dosing but had ready access to water. Each rat received a single oral dose of 10 grams/kg body weight of test compound by gastric intubation. Animals were observed for mortality and body weight changes for 14 days post-dosing. All surviving animals were sacrificed and necropsies were performed.

Results:

Value: LD50 > 10 g/kg

Number of deaths at each dose level: No deaths were observed

Remarks:

Sex	Initial Body Weight	Final Body Weight
M	265	330
M	265	299
M	276	338
M	272	319
M	272	335
F	248	284
F	223	257
F	247	282
F	206	232
F	222	244

All rats dosed with 10 grams/kg body weight survived the 14-day observation period. No signs of intoxication were seen during the observation period. The oral LD50 for the test material was determined to be greater than 10 grams/kg body weight. Body weight gain was within normal limits.

Gross autopsy findings revealed blanched and mottled kidneys in most rats.

Under the conditions of the test, the study material is not considered to be a toxic substance when administered by the oral route.

Reliability: (2) Reliable with restrictions Age of animals at the start of study and analytical composition were not reported.

Flag: Key study for SIDS endpoint.

References: Ethyl (1977) Toxicology Evaluation of Ethyl Compound 100-527. Gulf South Research Institute P.O. Box 1177 New Iberia, LA 70560 (unpublished report).

(3) **Test Substance**

Identity (purity): C18-C26 Alpha Olefin

Remarks: Blend of CAS No. 112-88-9, 1-Octadecene; CAS No. 3452-07-1, 1-Eicosene; CAS No. 1599-67-3, 1-Docosene; CAS No. 10192-32-2, 1-Tetracosene; CAS No. 18835-33-1, 1-Hexacosene (proportions unknown)

Method

Method/guideline: 16 CFR 1500.3 (c)(2)(i)
Type *(test type):* LD50
GLP: No
Year: 1977
Species/Strain: Rat/CFE
Sex: Male and female
No. of animals per sex per dose: 5

Vehicle: None specified
Route of administration: Oral gavage

Test Conditions: Ten healthy CFE rats (5M:5F) with body weights averaging approximately 250 grams were used to determine the oral toxicity of the test sample. Animals were fasted approximately 18 hours prior to dosing but had ready access to water. Each rat received a single oral dose of 10 grams/kg body weight of test compound by gastric intubation. Animals were observed for mortality and body weight changes for 14 days post-dosing. All surviving animals were sacrificed and necropsies were performed.

Results:

Value: LD50 > 10 g/kg
Number of deaths at each dose level: No deaths were observed

Remarks:

Sex	Initial Body Weight	Final Body Weight
M	289	358
M	290	342
M	264	313
M	283	340
M	279	296

F	218	248
F	222	257
F	224	260
F	234	266
F	219	262

All rats dosed with 10 grams/kg body weight survived the 14-day observation period. No signs of intoxication were seen during the observation period. The oral LD50 for the test material was determined to be greater than 10 grams/kg body weight. Body weight gain was within normal limits.

Gross autopsy findings revealed blanched and mottled kidneys in most rats.

Under the conditions of the test, the study material is not considered to be a toxic substance when administered by the oral route.

Reliability: (2) Reliable with restrictions. Age of test animals and analytical composition not reported.

References: Ethyl (1977) Toxicology Evaluation of Ethyl Compound 100-494. Gulf South Research Institute P.O. Box 1177 New Iberia, LA 70560 (unpublished report).

(4) Test Substance

Identity (purity): CAS 27070-58-2, Octadecene (C18 Alpha Olefin, Isomerized >98%, 20-30% branched, double bond randomized along carbon chain)

Method

Method/guideline: EPA OPP 81-1
Type *(test type):* LD50
GLP: Yes [X] No [ ]
Year: 1993
Species/Strain: Rat/HSD:SD
Sex: Males and females
No. of animals per sex per dose: 5

Vehicle: None
Route of administration: Oral gavage

Test Conditions: Single doses of 5050 mg/kg of undiluted test material were administered intragastrically to groups of 5 male and 5 female

fasted albino rats (young adults, 211-228 g [males], 194-208 g [females]). Animals were observed for 14 days. Individual body weights were recorded on Days 0, 7, and 14. A gross necropsy was performed on each animal at the termination of the study. Statistical methods were not used.

Results:

Value: LD50 > 5050 mg/kg

Number of deaths at each dose level: No deaths at 5050 ml/kg

Remarks: No deaths were observed. All animals gained weight during the study. Signs of toxicity included diarrhea in 1 male at 3 hours, and piloerection and polyuria in all animals, which were no longer evident in 4/5 males and 5/5 females by Day 5. One male exhibited piloerection until Day 11. The gross necropsy conducted on all animals at termination of the study revealed no observable abnormalities in any of the animals. The acute oral LD50 was greater than 5050 mg/kg.

Reliability: (1) Reliable without restrictions

References: Stillmeadow, Inc. (1993) C18 Alpha Olefin, Isomerized: Acute Oral Toxicity Study in Rats, Study No. 0486-93. Conducted for Chevron Chemical Company (unpublished report).

(5) Test Substance

Identity (purity): CAS No. 93924-10-8, C20-24 Alpha Olefin Fraction (carbon number C18 = max.5%; carbon number C20 = 45-60%; carbon number C22 = 30-50%; carbon number C24 = max.15%; carbon number C26 = max.1%)

Method

Method/guideline: Experimental
Type *(test type):* LD50
GLP: No
Year: 1990
Species/Strain: Conventional rat/Wistar
Sex: Males and females
No. of animals per sex per dose: 10

Vehicle: Olive oil
Route of administration: Oral gavage

Test Conditions: Single doses of 15.85 g/kg of test material diluted with olive oil (20% formulation) were administered intragastrically to groups of young adult rats, 140-160 g. Animals were observed for 14 days. A gross necropsy was performed on each animal at the termination of the study.

Results:

Value: LD50 > 15 g/kg

Number of deaths at each dose level: No deaths at 15.85 g/kg

Remarks: No signs of toxicity were seen. All animals gained weight during the study. The gross necropsy conducted on all animals at termination of the study revealed no observable abnormalities in any of the animals. The sample is nontoxic.

Reliability: (1) Reliable without restrictions

References: Research Institute of Organic Synthesis a.s (1990) Pardubice, Czech republic, Test No. T2102 (unpublished report).

(6) Test Substance

Identity (purity): CAS No. 93924-10-8, C20-24 Alpha Olefin (GULFTENE 20-24; Composition: <47% C20, <35% C22, <26% C24, <3% C18, <1% C16) ; 89.3% linear, 8.3% branched

Method

Method/guideline: Not specified
Type *(test type):* LD50
GLP: Yes [X] No [ ]
Year: 1982
Species/Strain: Rat/Fischer 344
Sex: Males and females
No. of animals per sex per dose: 5

Vehicle: corn oil
Route of administration: Oral gavage

Test Conditions: Animals were 14-19 weeks of age at study initiation. The test material was warmed to 37oC, diluted to 50% (w/v) with laboratory grade corn oil, and a dose equivalent to 5000 mg/kg of test substance was administered orally to 5 male and 5 female fasted rats. The animals received dose volumes of 2 ml/100g body weight. Body weights were recorded on Day 0 prior to dosing and on Days 7 and 14. All animals were observed for 14

days and a gross necropsy performed at study termination. No statistical analyses were performed.

Results:

Value:	LD50 > 5000 mg/kg
Number of deaths at each dose level:	No deaths at 5000 mg/kg
Remarks:	Clinical signs were limited to yellow staining of the inguinal region, oil around the mouth, and brown staining of the lower jaw; all had cleared by Day 5. No adverse findings were noted at necropsy. Throughout the study, no adverse effects were noted in body weight gains. The acute oral LD50 is greater than 5000 mg/kg.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Gulf Life Sciences Center (1982) Acute Oral Toxicity Test in Albino Rats Using Alpha Olefin Fraction C20-24, Report No. 82-030 (unpublished report).

(7) **Test Substance**

Identity (purity):	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 401
Type *(test type):*	LD50
GLP:	Yes [X] No [ ]
Year:	1998
Species/Strain:	Sprague-Dawley CD (Crl:CD®BR)
Sex:	Males and females
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Oral gavage
Statistical Methods:	The acute oral median lethal dose (LD50) was calculated by an accepted method, e.g. Weil (1952), Litchfield and Wilcoxon (1949), Finney (1971) or Thompson (1947)'s method. Where

possible LD50 values and 95% confidence limits were calculated for males and females separately.

Test Conditions: The test material was administered by oral gavage as a single limit dose of 5000 mg/kg body weight to a group of 10 fasted animals, 5 males and 5 females. Individual bodyweights were recorded prior to dosing on Day 0 and on Days 7 and 14 or at death. At the start of the main study the males weighed 206 to 222 g and the females 205 to 222 g and were approximately eight to twelve weeks old. Surviving animals were observed for 14 days after dosing and then sacrificed. All animals were subjected to a gross necropsy. The specific gravity of the test material was 0.796 and the dose volume was adjusted accordingly. This dose level was selected based upon data derived from a range-finding study of 1 male and 1 female.

Results:

Value: LD50 > 5000 mg/kg

Number of deaths at each dose level: One female was found dead one day after dosing.

Remarks: Surviving animals recovered 1 - 3 days after dosing. Clinical observations noted in all animals during the day of dosing were hunched posture and pilo-erection. Decreased respiratory rate and laboured respiration were noted in one female during the day of dosing. Hunched posture persisted in six animals (2 males and 4 females) one day after dosing, with ataxia noted in two females and tiptoe gait in one female. Hunched posture was noted in two females two days after dosing.

Abnormalities noted at necropsy of the female that died during the study were hemorrhagic lungs, dark liver and dark kidneys. No abnormalities were noted at necropsy of animals that were killed at the end of the study. Surviving animals showed expected gain in bodyweight during the study.

Reliability: (1) Reliable without restrictions

References: Driscoll R (1998) C20-24 Alkenes, Branched and Linear: Acute Oral Toxicity Study in The Rat, Project No. 703/116. Conducted by Safepharm Laboratories for Chevron Research and Technology Company (unpublished report).

(8) Test Substance

Identity (purity): CAS Nos. C22=1599-67-3, C24=10192-32-2, C26=18835-33-1, C28=18835-34-2: C22-28 Alpha Olefin

Remarks: (even-numbered carbons only; <4% C22, <76% C24-28, <20% C30+)

Method

Method/guideline:	Not specified
Type *(test type):*	LD50
GLP:	No
Year*:*	1967
Species/Strain:	Rat/Wistar
Sex:	Males
No. of animals per sex per dose:	10
Vehicle:	corn oil
Route of administration:	Oral gavage

Test Conditions*:* The solid olefin C22-28 blend was administered to 10 rats weighing between 200 and 235 grams as a 25% w/v solution in corn oil. An additional group of 10 rats weighing between 200 and 232 grams received 20 ml/kg of corn oil as an internal control. A group of 10 rats weighing between 203 and 226 grams received nothing and served as the sham control. Animals were observed for 14 days. Bodyweights were taken at 1, 2, 3, 4, 7, and 14 days. Necropsies were performed at study termination. Statistical methods were not used.

Results:

Value:	LD50 > 5000 mg/kg
Number of deaths at each dose level:	No deaths at 5000 mg/kg

Remarks: The acute oral LD50 was >5000 mg/kg. No significant gross pathology was seen. Several days after dosing, treated animals developed very coarse, oily fur over nearly the entire body. At study termination increased body weights were 55%, 58% and 46% for the sham control, vehicle control and treated groups, respectively.

Reliability: (2) Reliable with restrictions: The animals were not fasted and were dosed at volumes >10 ml/kg; and all required observation data are not presented.

References: Department of Occupational Health, Graduate School of Public Health, University of Pittsburgh, Pittsburgh, Pennsylvania (1967). Toxicological studies on several alpha olefins. Conducted for Gulf Research and Development Company, unpublished report.

(9) Test Substance

Identity (purity):	CAS Nos. C24=182636-05-1, C26=182636-06-2, C28=182636-07-3, C30=182636-08-4 : C24-30 Alkenes, Branched and Linear
Remarks:	even-numbered carbons only; <55% C24; <40% C26, <15% C28, <30% C30; 70%branched)

Method

Method/guideline:	OECD Guideline 401
Type *(test type):*	LD50
GLP:	yes
Year:	1998
Species/Strain:	Rat/Sprague-Dawley Crl:CD®BR
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	peanut oil
Route of administration:	Oral gavage
Statistical methods:	The acute oral median lethal dose (LD50) was calculated by an accepted method, e.g. Weil (1952), Litchfield and Wilcoxon (1949), Finney (1971) or Thompson (1947)'s method. Where possible LD50 values and 95% confidence limits were calculated for males and females separately.
Test Conditions:	A study was performed to assess the acute oral toxicity of the test material in the Sprague-Dawley strain rat. Following a range-finding study, a group of ten fasted animals (five males and five females) was given a single oral dose of undiluted test material at a dose level of 5000 mg/kg bodyweight. At the start of the study, the males weighed 216 to 236g and the females 204 to 230g and were approximately ten to fourteen weeks old. The animals were observed for fourteen days after the day of dosing and were then killed and subjected to gross necropsy.

Results:

Value:	LD50 > 5000 mg/kg
Number of deaths at each dose level:	No deaths at 5000 mg/kg
Remarks:	No signs of systemic toxicity were noted during the study. All surviving animals showed expected weight gain during the study. Surviving animals showed no abnormalities at necropsy.
	The acute oral median lethal dose (LD50) of the test material in the Sprague-Dawley strain rat was found to be greater than 5000 mg/kg bodyweight.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Driscoll R, (1998) Acute Oral Toxicity Study in The Rat with C24-30 Alkenes, Branched and Linear. Study No. 703/130. Conducted by SafePharm Laboratories Limited for Chevron Research and Technology Company (unpublished report).

(10) Test Substance

Identity (purity): CAS No. 131459-42-2, Alkene, C24-54 Branched and Linear, Alpha (even-numbered carbons); (C30+) 8.0% C24-28, 92% >C30; 50% of molecules are branched with even carbon numbers (C2-26) of vinylidene isomers at 2nd carbon.

Method

Method/guideline:	Not specified
Type *(test type):*	LD50
GLP:	Yes [X] No [ ]
Year:	1982
Species/Strain:	Rat/Fischer 344
Sex:	Males and females
No. of animals per sex per dose:	5 each for treatment; 3 males and 2 females for procedural control
Vehicle:	none
Route of administration:	Oral gavage

Test Conditions: C30+ Alpha Olefin was formed into dosing pellets by heating to its melting point, drawing it into a thin-walled plastic tube, allowing it to solidify and extruding the solid pellets. Fisher 344 albino rats (5 male and 5 female) were anesthetized with approximately 40 mg/kg of Ketamine hydrochloride given intramuscularly. A thin-walled plastic tube was then inserted down the animal's esophagus and pellets of test material were pushed through the tube and into the animal's stomach using a wooden applicator stick. Three males and two females served as a procedural control group. The dose level was 2000 mg/kg. The animals were observed for 14 days. No statistical analyses were performed on the data.

Results:

Value:	LD50 > 2000 mg/kg
Number of deaths at each dose level:	No treatment-related deaths at 2000 mg/kg

Remarks: In a pre-test study, two males were administered 5000 mg/kg of test substance. The animals died due to physical overloading of the digestive system, therefore, 2000 mg/kg was selected as the dose level for the definitive study.

In the 2000 mg/kg dose group, one female died on day two due to trauma resulting from the dosing procedure. No adverse effects were noted in body weight gains among the surviving test and control animals. All animals exhibited impaired coordination in the first three hours following dosing. This reaction was due to the residual effects of the anesthetic. No remarkable findings were noted among the control animals throughout the remainder of the observational period. Clinical observations consisted of yellow staining of the inguinal region in five animals, yellow staining around the mouth in three animals, and labored respiration and excessive salivation in one animal (sex of animals is not available). These findings cleared in two days. While no adverse effects that could be attributed to test material administration were noted at necropsy, the following observations were made: five animals had congestion in their left sub-lumbar lymph nodes, one animal had a small white object lodged in its stomach, one animal had an empty stomach, and one animal had congestion in the upper 1 cm of its duodenum. For the control group, one animal had congestion in its left sub-lumbar lymph node, one animal had a congested thymus, and one animal had no gastro-intestinal contents (sex of animals is not available).

All deaths that occurred during the conduct of the study were attributed to trauma and therefore did not contribute to the toxicity of the compound. The acute oral LD50 for Alpha Olefin C30+ was determined to be greater than 2000 mg/kg.

Reliability: (2) Reliable with restrictions: This study meets the current OECD 401 guideline with restrictions due to the non-standard dosing procedure and the administration of an anesthetic.

References: Gulf Life Sciences Center (1982) Acute Oral Toxicity Test in Albino Rats Using Alpha Olefin C30+, Report No. 82-038 (unpublished report).

(11) Test Substance

Identity (purity): CAS# 131459-42-2, Alpha-olefin fraction C24-54 (C30+);
Purity: carbon number C28 and lower max.28%
carbon number C30+ min.72%, 33-39% branched, >50% linear alpha olefin, 10% internal olefins

Method

Method/guideline:	Experimental
Type *(test type):*	LD50
GLP:	No
Year:	1990
Species/Strain:	Conventional rat/Wistar
Sex:	Males and females
No. of animals per sex per dose:	10
Vehicle:	Olive oil
Route of administration:	Oral gavage
Test Conditions:	Single doses of 15.85 g/kg of test material diluted with olive oil (20% formulation) were administered intragastrically to groups of young adult rats, 140-157 g. Animals were observed for 14 days. A gross necropsy was performed on each animal at the termination of the study.
Results:	
Value:	LD50 > 15 g/kg
Number of deaths at each dose level:	No deaths at 15.85 g/kg
Remarks:	No signs of toxicity were seen. All animals gained weight during the study. The gross necropsy conducted on all animals at termination of the study revealed no observable abnormalities in any of the animals. The sample is nontoxic.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Research Institute of Organic Synthesis a.s (1990) Pardubice, Czech republic, Test No. T2103 (unpublished report).

B. Acute inhalation toxicity

Test Substance

Identity (purity):	C16-C18 Alpha Olefin (CAS No. 629-73-2, 1-Hexadecene; CAS No. 112-88-9, 1-Octadecene) (proportion unknown)

Method

Method/guideline:	Not specified
Type *(test type):*	LC50
GLP:	Yes [ ] No [X]

Year:	1973
Species/Strain:	Rat/Sprague-Dawley
Sex:	Males
No. of animals per sex per dose:	10
Vehicle:	None
Route of administration:	Inhalation

Test Conditions: Ten male rats weighing between 200 and 300 g were exposed for 1 hour or 4 hours to saturated vapor at ambient temperature of the test substance and observed for 14 days. The number of animals per group was not reported. The animals were observed for toxic signs during exposure and during the 14-day observation period. On the 14th day, they were sacrificed for the determination of gross pathological changes.

The inhalation atmosphere was generated by bubbling chamber air through undiluted test material. Air flow was 2.9 L/min. Nominal concentrations were reported as >0 mg/L for the one hour exposure and >0.06 mg/L for the 4-hour exposure. No further experimental details were reported.

Results:

Value:	LC50 > the saturated vapor concentration for one and four hour exposures
Number of deaths at each dose level:	None

Remarks: There were no signs of toxicity during exposure or during the 14-day observation period. Necropsy did not reveal any gross pathological changes.

Reliability: (4) Not assignable: Only limited details of procedures were reported.

References: Ethyl Corporation (1973) (unpublished report).

C. Acute dermal toxicity

(1) Test Substance

Identity (purity): C18-C24 Alpha Olefin

Remarks: Blend of CAS No. 112-88-9, 1-Octadecene; CAS No. 3452-07-1, 1-Eicosene; CAS No. 1599-67-3, 1-Docosene; CAS No. 10192-32-2, 1-Tetracosene (proportions unknown)

Method

Method/guideline: 16 CFR 1500.40 & CFR 1500.3 (c)(1)(ii) (c) (2) (iii)
Type (test type): LD50
GLP: No
Year: 1977
Species/Strain: Rabbits/New Zealand White
Sex: Males and females
No. of animals per sex per dose: 3

Vehicle: None specified
Route of administration: Dermal

Test Conditions: Six healthy New Zealand albino rabbits (3M:3F) were used to evaluate the toxicity of the test material following dermal application of 10 grams/kg body weight. Prior to application of test material, the animals were prepared by shaving the application site and abrading the skin every two to three centimeters longitudinally over one-half the exposure area. Test material was held in contact with the skin by means of saran wrap covered with brown paper for 24 hours. Animals were observed for mortality and general behavior for 14 days post dosing. On the 14th day all surviving animals were sacrificed and necropsies were performed.

Results:

Value: LD50 > 10 g/kg
Number of deaths at each dose level: None

Remarks:

Sex	Initial Body weight	Final body weight
M	2400	2600
M	2700	3300
M	2300	2850
F	2600	2550
F	2600	3150
F	2300	2800

All rabbits dosed with 10 grams/kg body weight survived the 14-day observation period. The dermal LD50 for the test material was determined to be greater than 10 grams/kg body weight. Five out of the six animals had satisfactory weight gain during the study. One female rabbit had a slight decrease in body weight. Under the conditions of the test, the study material is not considered to be a toxic substance when administered by the dermal route.

Reliability: (2) Reliable with restrictions age of animals and compositional analysis not reported

Flag: Key study for SIDS endpoint

Reference: Ethyl (1977) Toxicology Evaluation of Ethyl Compound 100-527. Gulf South Research Institute P.O. Box 1177 New Iberia, LA (unpublished report).

(2) Test Substance

Identity (purity): C18-C26 Alpha Olefin

Remarks: Blend of CAS No. 112-88-9, 1-Octadecene; CAS No. 3452-07-1, 1-Eicosene; CAS No. 1599-67-3, 1-Docosene; CAS No. 10192-32-2, 1-Tetracosene; CAS No. 18835-33-1, 1-Hexacosene (proportions unknown)

Method

Method/guideline:	16 CFR 1500.40 & CFR 1500.3 (c)(1)(ii) (c) (2) (iii)
Type (test type):	LD50
GLP:	No
Year:	1977
Species/Strain:	Rabbits/New Zealand White
Sex:	Males and females
No. of animals per sex per dose:	3
Vehicle:	None specified
Route of administration:	Dermal

Test Conditions: Six healthy New Zealand albino rabbits (3M:3F) were used to evaluate the toxicity of the test material following dermal application of 10 grams/kg body weight. Prior to application of test material, the animals were prepared by shaving the application site and abrading the skin every two to three centimeters longitudinally over one-half the exposure area. Test material was held in contact with the skin by means of saran wrap covered with brown paper for 24 hours. Animals were observed for mortality and general behavior for 14 days post dosing. On the 14th day all surviving animals were sacrificed and necropsies were performed.

Results:

Value:	LD50 > 10 g/kg
Number of deaths at each dose level:	None

Remarks:

Sex	Initial Body weight	Final Body weight
M	2550	3000
M	2800	3150
M	2450	2950
F	2400	2950
F	2200	2800
F	2350	2750

All rabbits dosed with 10 grams/kg body weight survived the 14-day observation period. The dermal LD50 for the test material was determined to be greater than 10 grams/kg body weight. All six animals had satisfactory weight gain during the study. Under the conditions of the test, the study material is not considered to be a toxic substance when administered by the dermal route.

Reliability: (2) Reliable with restrictions. Age of animals and compositional analysis was not reported

Reference: Ethyl (1977) Toxicology Evaluation of Ethyl Compound 100-494. Gulf South Research Institute P.O. Box 1177 New Iberia, LA (unpublished report).

(3) Test Substance

Identity (purity): CAS 27070-58-2, Octadecene (C18 Alpha Olefin, Isomerized >98%, 20-30% branched, double bond randomized along carbon chain)

Method

Method/guideline: EPA OPP 81-2
Type *(test type):* LD50
GLP: Yes
Year: 1993
Species/Strain: Rabbit/New Zealand white
Sex: Males and females
No. of animals per sex per dose: 5

Vehicle: None
Route of administration: Dermal

Test Conditions: The objective of this study was to determine the acute dermal toxicity potential of the test material. Each animal was prepared on the day prior to treatment by clipping the dorsal surface of the trunk free of hair to expose not less than 10% of the total body

surface area. Five albino rabbits of each sex (young adult [3-6 mos] weighing 2.400-2.725 kg [males] and 2.400-2.950 kg [females]) were treated with a single dermal application of 2020 mg/kg of undiluted test material for 24 hours. The treated area was covered with gauze and a semi-permeable dressing (orthopedic stockinette) to retard evaporation of volatile substances and to prevent possible ingestion of the test material. After 24 hours the wrappings and gauze were removed from the animals. The exposed areas were gently washed with room temperature tap water and a clean wet cloth was used to remove as much remaining test material as possible. Animals were observed for pharmacologic and/or toxicologic signs including signs of dermal irritation frequently throughout the study. Individual body weights were recorded on Days 0, 7, and 14. A gross necropsy was conducted on each animal at the termination of the study. Statistical methods were not used.

Results:

Value:	LD50 > 2020 mg/kg
Number of deaths at each dose level:	There were no mortalities
Remarks:	Four animals of each sex lost weight or failed to gain weight between Days 7 and 14. A single female animal had diarrhea on Days 9 and 10. The gross necropsy conducted on each animal at termination of the study revealed no observable abnormalities in any of the animals. The acute dermal LD50 was greater than 2020 mg/kg.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Stillmeadow, Inc. (1993) Acute Dermal Toxicity Study in Rabbits, Study No. 0487-93. Conducted for Chevron Chemical Company (unpublished report).

(4) Test Substance

Identity (purity):	CAS No. 93924-10-8, C20-24 Alpha Olefin Fraction (carbon number C18 = max.5%; carbon number C20 = 45-60%; carbon number C22 = 30-50%; carbon number C24 = max.15%; carbon number C26 = max.1%)

Method

Method/guideline:	Experimental
Type *(test type)*:	LD50
GLP:	No

Year:	1990
Species/Strain:	Conventional Rat, Wistar
Sex:	Males
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Dermal
Test Conditions:	Sample was applied at a quantity of 5ml/kg on the shaved skin, area 4 x 6cm, of the rat's back. The sample was in contact with skin for 24 hrs, fixed by gauze, aluminum foil and plaster bandage, so that the animals were able to move freely and couldn't eat the sample. The bandage was removed after 24 hrs. Rats were observed for the next 14 days, after which rats were weighed, euthanized, and necropsied and organs were macroscopically examined.

Results:

Value:	LD50 > 5 ml/kg
Number of deaths at each dose level:	There were no mortalities
Remarks:	No clinical signs of toxicity were noted. There was normal body weight increase. No macroscopic pathomorphological changes were found during the necropsies. The results indicate that the C20-24 fraction is not absorbed in toxic quantity.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Research Institute of Organic Synthesis a.s (1990) Pardubice, Czech Republic, Test No. T2102 (unpublished report).

(5) Test Substance

Identity (purity):	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 402
Type *(test type)*:	LD50

GLP:	Yes
Year:	1998
Species/Strain:	Rat/Sprague-Dawley CD (Crl:CD®BR)
Sex:	Males and females
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Dermal
Statistical Methods:	The acute dermal median lethal dose (LD50) was calculated by an accepted method, e.g. Weil (1952), Litchfield and Wilcoxon (1949), Finney (1971) or Thompson (1947)'s method. Where possible LD50 values and 95% confidence limits were calculated for males and females separately.
Test Conditions:	A study was performed to assess the acute dermal toxicity of the test material in the Sprague-Dawley strain rat. A group of ten animals (five males and five females) was given single, 24-hour, semi-occluded, dermal applications to intact skin at a dose level of 2000 mg/kg bodyweight. The specific gravity of the test material was 0.796 and the dose volume was adjusted accordingly. At the start of the main study the males weighed 206 to 225 g and the females 206 to 224 g and were approximately eight to twelve weeks old. The animals were observed for fourteen days after the day of treatment and were then killed for gross pathological examination.
Results:	
Value:	LD50 > 2000 mg/kg
Number of deaths at each dose level:	There were no deaths
Remarks:	No signs of systemic toxicity or skin irritation were noted during the study. All animals showed expected gain in bodyweight during the study. No abnormalities were noted at necropsy. The acute dermal median lethal dose (LD50) of the test material in the Sprague-Dawley strain rat was found to be greater than 2000 mg/kg bodyweight.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Driscoll R (1998) C20-24 Alkenes, Branched and Linear: Acute Dermal Toxicity Study in The Rat, SafePharm Laboratories Limited Project No. 703/117. Conducted for Chevron Research and Technology Company (unpublished report).

(6) **Test Substance**

Identity (purity):	CAS# 131459-42-2, Alpha-olefin fraction C24-54 (C30+), Purity: carbon number C28 and lower max.28% carbon number C30+ min.72%, 33-39% branched, >50% linear alpha olefin, 10% internal olefins

Method

Method/guideline:	Experimental
Type *(test type):*	LD50
GLP:	No
Year:	1990
Species/Strain:	Conventional Rat, Wistar
Sex:	Males
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Dermal
Test Conditions:	Sample was applied at a quantity of 5ml/kg on the shaved skin, area 4 x 6cm, of the rat's back. The sample was in contact with skin for 24 hrs, fixed by gauze, aluminum foil and plaster bandage, so that the animals were able to move freely and couldn't eat the sample. The bandage was removed after 24 hrs. Rats were observed for the next 14 days, after which rats were weighed, euthanized, and necropsied and organs were macroscopically examined.

Results:

Value:	LD50 > 5 ml/kg
Number of deaths at each dose level:	There were no mortalities
Remarks:	No clinical signs of toxicity were noted. There was normal body weight increase. No macroscopic pathomorphological changes were found during the necropsies. The results indicate that the C30+ fraction is not absorbed in toxic quantity.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Research Institute of Organic Synthesis a.s. (1990) Pardubice, Czech Republic, Test No. T2103 (unpublished report).

D. Acute toxicity, other routes

No data available

5.3 Corrosiveness/Irritation

A. Skin Irritation/Corrosion

(1) **Test Substance:** CAS No. 112-88-9, 1-Octadecene (~92%, GULFTENE 18)

pH: Not applicable

Method: OECD 404

Test Type: in vivo
GLP: Yes
Year: 1995

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Male and female
Number of animals per sex per dose: 5 males and 1 female

Total dose: 0.5 ml
Vehicle: None
Exposure time period: 4 hrs
Grading scale: Draize

Method Remarks: At the start of the study, the animals weighed 2.48 to 2.85 kg and were approximately 12 to 20 weeks old. One-half ml undiluted material was applied to the unabraded skin on the shaved backs of 6 rabbits, under a semi-occluded dressing (cotton gauze patch placed in position with a strip of porous tape; trunk wrapped in an elasticated corset [TUBIGRIP]). A contralateral area of untreated skin was identified to serve as the control against which the reactions of the untreated site were evaluated. Four hours after application, the corset and patches were removed and residual test material was removed by swabbing with cotton wool soaked in 74% Industrial Methylated Spirits. The control sites were similarly swabbed. Scores were made for erythema and edema at 0.5, 24, 48, 72 and 96 hr after removal of patches, and at 7 and 14 days after initiation of exposure.

Results: The 4-hr exposure produced very slight erythema at 5 treated skin sites with well-defined erythema at one treated skin site at the 30-

minute observation. Very slight erythema was also apparent at 2 control sites at this time. Very slight erythema persisted at 3 treated skin sites with well-defined erythema apparent at 3 treated skin sites at the 24, 48 and 72-hr observations. Very slight erythema was noted at 4 treated skin sites with well-defined erythema at 2 treated skin sites at the 96-hr observation. Desquamation was noted at 5 treated sites at the 96-hr observation. Crust formation was apparent at 2 treated skin sites at the 7-day observations. The dermal reactions extended up to 4 cm beyond all treated skin sites during the study. Very slight edema was noted at 4 treated sites at the 30-minute observation and at 3 treated sites at the 24-hr observation. Slight edema was noted at 2 treated sites at the 24, 48 and 72-hr observations and persisted at 1 site at the 96-hr observation. The Draize primary irritation index was 2.29. The mean 24-72 hr scores for erythema and edema were 1.5 and 0.9, respectively.

Reliability: (1) Reliable without restrictions

Reference: Driscoll, R. (1996) Acute dermal irritation test in the rabbit with GULFTENE 18, Report 703/081. Conducted by Safepharm Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

(2) **Test Substance:** CAS No. 112-88-9, 1-Octadecene (NEODENE 18)

pH: Not applicable

Method: US EPA TSCA (40 CFR)

Test Type: in vivo
GLP: Yes
Year: 1991

Test Conditions

Species: Rabbits
Strain:
Cell type:
Sex: Male and female
Number of animals per sex per dose: 3

Total dose: 0.5 ml
Vehicle: None
Exposure time period: 4 hr
Grading scale: Draize

	Method Remarks:	Groups of 3 males and 3 females. Doses of 0.5 ml undiluted material applied under occlusive dressing for 4 hours. Scored at 0.5, 1, 24, 48 and 72 hours and on Day 7 (termination).
	Results:	Primary Irritation Index = 3.2. Mean 24, 48 and 72-hour scores: erythema 2.17; oedema 0.94. Mean scores on Day 7: erythema 0.33; oedema 0.94.
	Reliability:	(2) Reliable with restrictions; the testing guideline specifies a semi-occlusive dressing, but an occlusive dressing was used.
	Reference:	Shell Oil Company (1991) Primary skin irritation study in rabbits of Neodene 18 alphaolefin. Ref. 91-8383-21 (unpublished report).
(3)	**Test Substance:**	CAS No. 112-88-9, 1-Octadecene (NEODENE 18)
	pH:	Not applicable
	Method:	Human Patch Test
	Test Type:	in vivo
	GLP:	No
	Year:	1992
	Test Conditions	
	Species:	Human volunteers
	Strain:	
	Cell type:	
	Sex:	Male and female
	Number of animals per sex per dose:	12 females and 6 males
	Total dose:	0.2 ml of undiluted, 25%, 10%, and 1% dilutions in mineral oil
	Vehicle:	mineral oil
	Exposure time period:	24 hr
	Grading scale:	See Method Remarks
	Method Remarks:	Each person received a single 24 hour semi-occluded patch exposure to 0.2 ml undiluted product and 25, 10 and 1% dilutions in mineral oil to the upper arm. Test sites were scored at 30 minutes and 24 hours after patch removal. Scores of 0-3 were given to reactions at both time points and these were summed to give a maximum of 6. Sodium lauryl sulphate (SLS) in distilled water was included as control.

Results: No evidence of irritation was noted with dilute applications of Neodene 18 (mean score 0.0). Undiluted Neodene 18 caused a strong clinical reaction. At the 30 minute observation time, 16 of the 18 volunteers exhibited moderate to strong erythema, oedema and papules. At 24 hours, 17 subjects showed similar signs and 9 of these had effects spreading beyond the application site. The mean score was 4.28. Two subjects showed mild to moderate erythema to 0.25% SLS (mean score 0.22).

Reliability: (2) Reliable with restrictions; exposure time was too long

Reference: Shell Oil Company (1992) Evaluation of primary irritation potential of Neodene 18 in humans. Single 24 hour application. Report 92-1388-70A. (unpublished report).

(4) Test Substance: CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

pH: Not applicable

Method: OECD 404 except that only 3 animals were employed

Test Type: in vivo
GLP: Yes
Year: 1994

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Male and female
Number of animals per sex per dose: 2 males and 1 female

Total dose: 0.5 ml
Vehicle: None
Exposure time period: 4 hr
Grading scale: Draize

Method Remarks: At the start of the study, the animals (young adults) weighed 2.0 to 3.5 kg. One-half ml undiluted material was applied to the unabraded skin (approximately 6.25 cm^2) on the shaved backs of 3 rabbits, under a semi-occluded dressing (cotton gauze patch covered with porous tape; trunk loosely wrapped with a sheet of Texwipe® cotton cloth). Each rabbit was fitted with an Elizabethan collar during the exposure period. A contralateral area of untreated skin served as the control against which reactions of the treated site

were evaluated. After 4 hrs, patches were removed and residual test substance was removed using a paper towel moistened with tap water. Scores were made for erythema and edema at 1, 24, 48 and 72 hr, and at 7 and 14 days after initiation of exposure.

Results: The 4-hr exposure produced well-defined erythema and very slight to slight edema which cleared by day 14. No physical or behavioral abnormalities were observed in any animal. The Draize primary irritation index was 2.2/8. The average of 24-72 scores were 1.3, 2.0, and 1.3 for erythema and 0.0, 0.3, and 0.3 for edema for each animal.

Reliability: (1) Reliable without restrictions

Reference: Morris, T. (1995) Acute dermal irritation screening study in rabbits with C16/C18 Alpha Olefins, Isomerized. Conducted by Hill Top Biolabs, Inc., Project No. 94-8345-21 (A), for Chevron Research and Technology Company (unpublished report).

(5) **Test Substance:** CAS No. 93924-10-8, C20-24 Alpha Olefin (NEODENE 20-24)

pH: Not applicable

Method: US EPA TSCA (40 CFR)

Test Type: in vivo
GLP: Yes
Year: 1991

Test Conditions

Species: Rabbits
Strain:
Cell type:
Sex: Male and female
Number of animals per sex per dose: 3

Total dose: 0.5 ml
Vehicle: None
Exposure time period: 4 hr
Grading scale: Draize

Method Remarks: Groups of 3 males and 3 females. Doses of 0.5 ml undiluted material applied under occlusive dressing for 4 hours. Scored at 0.5, 1, 24, 48 and 72 hours and on Day 7 (termination).

Results: Primary Irritation Index = 2.7. Mean 24, 48 and 72-hour scores: erythema 1.94; oedema 0.72. Mean scores on Day 7: erythema 0.33; oedema 0.0.

Reliability: (2) Reliable with restrictions; the testing guideline specifies a semi-occlusive dressing, but an occlusive dressing was used.

Reference: Shell Oil Company (1991) Primary skin irritation study in rabbits of Neodene 20-24 alpha olefin. Ref. 91-8384-21 (unpublished report).

(6) **Test Substance:** CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only)
(<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

pH: Not applicable

Method: OECD 404

Test Type: in vivo
GLP: Yes
Year: 1997

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Male
Number of animals per sex per dose: 6 males

Total dose: 0.5 ml
Vehicle: None
Exposure time period: 4 hrs
Grading scale: Draize

Method Remarks: At the start of the study, the animals weighed 2.46 to 2.71 kg and were approximately 12 to 20 weeks old. One-half ml undiluted material was applied to the unabraded skin on the shaved backs of 6 rabbits, under a semi-occluded dressing (cotton gauze patch placed in position with a strip of porous tape; trunk wrapped in an elasticated corset [TUBIGRIP]). A contralateral area of untreated skin was identified to serve as the control against which the reactions of the untreated site were evaluated. Four hours after application, the corset and patches were removed and residual test material was removed by swabbing with cotton wool soaked in

liquid paraffin. The control sites were similarly swabbed. Scores were made for erythema and edema at 0.5, 24, 48, and 72 hr after removal of patches.

Results: The 4-hr exposure produced no dermal irritation during the 72-hr observation period. The Draize primary irritation index was 0.0. The mean 24-72 hr scores for erythema and edema were 0.0 and 0.0, respectively.

Reliability: (1) Reliable without restrictions

Reference: Driscoll, R. (1998) Acute dermal irritation test in the rabbit with C20-C24 Alkenes, Branched and Linear, Report 703/118. Conducted by Safepharm Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

B. Eye Irritation/Corrosion

(1) Test Substance: C18-24 Alpha Olefin

Remarks: Blend of CAS No. 112-88-9, 1-Octadecene; CAS No. 3452-07-1, 1-Eicosene; CAS No. 1599-67-3, 1-Docosene; CAS No. 10192-32-2, 1-Tetracosene (proportions unknown)

pH: Not applicable

Method: USA 16 CFR 1500.42

Test Type: in vivo
GLP: No
Year: 1977

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Not reported
Number of animals per dose: 6

Dose(s) used: 0.1 ml
Vehicle: None
Observation period: 72 hrs
Scoring method used: Draize scoring at 24, 48, and 72 hours after treatment

Remarks: Six New Zealand white rabbits had 0.1 ml material applied to right eye. Eyes were not irrigated. Observations were made at 24, 48, and 72 hours.

Results: All rabbits had mild conjunctivitis that cleared in 2 days. No corneal opacity occurred. At 24 hours, 1 rabbit had scores of 2 for redness and edema, 5 animals had scores of 1. At 48 hours, 2 animals had scores of 1 for redness, 1 animal had a score of 2 and 2 animals had scores of 1 for swelling. At 72 hours, all scores were 0. Mean Draize score = 4.67/110 at 24 hr; 2.0 at 48 hr; 0 at 72 hr; mean 24-72-hr scores for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis were 0, 0, 0.50, and 0.61, respectively.

Reliability: (2) Reliable with restrictions composition and sex of test animals was not reported.

Reference: Gulf South Research Institute, New Iberia, Louisiana (1977) Toxicological Evaluation of Ethyl Compound 100-527 Prepared for Ethyl Corporation (unpublished report).

(2) **Test Substance:** CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

pH: Not applicable

Method: OECD 405 except that only 3 animals were used

Test Type: in vivo
GLP: Yes
Year: 1994

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Male and females
Number of animals per dose: 1 male and 2 females

Dose(s) used: 0.1 ml
Vehicle: None
Observation period: 72 hrs
Scoring method used: Draize scoring at 1, 24, 48, and 72 hours after treatment

Remarks: Young adult rabbits weighing 3.005 to 3.079 kg were used. The undiluted test substance was applied to one eye of each animal. The lids were gently held together for approximately one second. The eyes were rinsed after 24 hours. The eyes were examined for ocular irritation at 1, 24, 48 and 72 hrs following treatment. With the exception of the 1 hr scoring, all eyes were scored again for

corneal opacity, intensity, and area using sodium fluorescein. Each animal was also observed daily for any physiological or behavioral abnormalities.

Results: Draize score at 24 hours was 2.0/110 for eyes scored with and without sodium fluorescein. The average of the 24-72 hr scores for each animal were 0 for corneal opacity and iritis; 0.0, 0.33, and 0.33 for conjunctival redness, and 0.0, 0.33, and 0.0 for conjunctival chemosis.

Remarks: The test substance did not produce corneal opacity or iritis but did produce conjunctival irritation which was observed at the 1 and 24-hr readings. All eyes were clear at the 48-hr reading. The maximum total irritation score observed for individual animals was 4.

Reliability: (1) Reliable without restrictions

Reference: Morris, T. (1995) Acute eye irritation screening study in rabbits with C16/C18 Alpha Olefins, Isomerized. Conducted by Hill Top Biolabs, Inc., Project No. 94-8346-21 (A), for Chevron Chemical Company (unpublished report).

(3) **Test Substance:** CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only)
(<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

pH: Not applicable

Method: OECD 405

Test Type: in vivo
GLP: Yes
Year: 1997

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Male and females
Number of animals per dose: 3 per sex for unwashed group; 2 females and 1 male for washed group

Dose(s) used: 0.1 ml
Vehicle: None

Observation period:	72 hrs
Scoring method used:	Draize scoring at 1, 24, 48, and 72 hours after treatment
Remarks:	Young adult rabbits weighing 2.48 to 2.93 kg and approximately 12-16 weeks old were used. The undiluted test substance was applied to one eye of each of 6 animals. The lids were gently held together for approximately one second. To minimize pain on instillation of the test material, one drop of local anesthetic (0.5% proxymetacaine hydrochloride) was instilled into both eyes 1 to 2 minutes before dosing. A second group of 3 animals was treated in a similar manner, except that the treated eyes were gently irrigated with 100 mL of lukewarm tap water for one minute 30 seconds following introduction of the test material. The eyes were examined for ocular irritation at 1, 24, 48 and 72 hrs following treatment. Each animal was also observed daily for any physiological or behavioral abnormalities.
Results:	Draize score at 24 hours was 0.0/110 for eyes scored with and without washing. The averages of the 24-72 hr scores were 0 for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis.
Remarks:	The test substance did not produce corneal opacity or iritis but did produce conjunctival irritation which was observed at the 1-hr reading (unwashed: 3/6 animals; washed: 2/3 animals). All eyes were clear at the 24-hr reading.
Reliability:	(1) Reliable without restrictions
Reference:	Driscoll, R. (1998) Primary eye irritation test in the rabbit with C20-C24 Alkenes, Branched and Linear, Report 703/119. Conducted by Safepharm Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

5.4 Skin Sensitisation

A. Test Substance: CAS No. 112-88-9, 1-Octadecene (NEODENE 18 Alpha Olefin)

Method: Buehler, 1965; Ritz and Buehler, 1980

Test Type:	challenge
GLP:	Yes
Year:	1992

Test Conditions

Species:	Guinea pig
Strain:	No data
Sex:	No data
Number of animals	

per sex per dose: 20 test and 10 control, sex unknown
Route of administration: Topical
Induction conc.: 5%
Induction vehicle: Acetone
Challenge conc.: 2.5%
Challenge vehicle: Acetone
Grading system used: Buehler
0=no reaction
+/--= slight, patchy erythema
1=slight but confluent, or moderate patchy erythema
2=moderate erythema
3=severe erythema with or without edema

Method remarks: Guinea pig, 20 test and 10 control animals. Groups of guinea pigs were treated with either 0.5 ml test material in diluent, 0.5 ml 0.1% w/v 2,4-dinitrochlorobenzene (DNCB positive control) or 0.5 ml ethanol (diluent control). Shaved sites were treated topically under an occlusive dressing 1 day/week, 6 hr/day for 3 consecutive weeks. After a 2 week rest, a challenge dose was given at the original site and a virgin site. Also at this time, a separate group was treated with 0.5 ml test material at the same concentration as used in the induction treatments. This was to measure irritation. Scoring was carried out 24 and 48 hr later.

Results: Negative for sensitization

Results Remarks:

	24 hr scores	48 hr scores
test group	7/20 at grade +/-	6/20 at grade +/-
control	5/10 at grade +/-	6/10 at grade +/-

Reliability: (1) Reliable without restrictions

Reference: Shell Oil Company (1992) Delayed contact hypersensitivity study in guinea pigs (Buehler technique): Neodene 18 alpha olefin. Ref 91-8383-21(B) (unpublished report).

Buehler, E.V. (1965) Delayed contact hypersensitivity in the guinea pig, *Archives of Dermatology* 91:171-177.

Ritz, H.L. and E.V. Buehler (1980) Planning, conduct and interpretation of guinea pig sensitization patch tests in *Current Concepts in Cutaneous Toxicity*, ed. V. Drill and P. Lazar. Academic Press, New York, N.Y. pp. 25-42.

B. Test Substance: CAS No. 112-88-9, 1-Octadecene (NEODENE 18 Alpha Olefin)

Method: Human Patch Test
Test Type: challenge

GLP:	No
Year:	1992

Test Conditions

Species:	Human volunteers
Strain:	
Sex:	Male and female
Number of animals per sex per dose:	31 females and 5 males
Route of administration:	Topical
Induction conc.:	25%
Induction vehicle:	Mineral oil
Challenge conc.:	25%
Challenge vehicle:	Mineral oil
Grading system used:	No data
Method remarks:	Each subject received 0.2 ml of test material in a semi-occluded patch exposure of 24 hours on 3 alternate days for 3 weeks (9 induction exposures). After 10-17 days rest, challenge applications were given at a test site and a naive site on the upper arm for 24 hours. Sodium lauryl sulphate (SLS) at 0.1% in water was included as control.
Results:	Negative for sensitization
Grades:	No data
Remarks:	Two subjects developed a transient reaction to NEODENE 18 during the induction phase whilst eight subjects reacted to the SLS. There was no reaction to either NEODENE 18 or to SLS challenge.
Reliability:	(1) Reliable without restrictions
Reference:	Shell Oil Company (1992) Repeated insult patch test of NEODENE 18 in humans. Report No. 92-1388-70B. (unpublished report).

C. **Test Substance:** CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

Method: Buehler

Test Type:	challenge
GLP:	Yes
Year:	1994

Test Conditions

Species:	Albino guinea pig
Strain:	Hartley
Sex:	Males and females
Number of animals per sex per dose:	1st Pilot (4 doses) = 1, 2nd Pilot (4 doses) = 1, Induction = 10, Challenge = 5, Rechallenge = 5
Route of administration:	Topical
Induction conc.:	5% for test substance
Induction vehicle:	Mineral Oil Light U.S.P. for test substance, 95% ethyl alcohol for positive control
Challenge conc.:	5% for test substance
Challenge vehicle:	Mineral Oil Light U.S.P. for test substance, acetone for positive control
Grading system used:	0 = no reaction, ± = slight, patchy erythema, 1 = slight but confluent, or moderate patchy erythema, 2 = moderate erythema, 3 = severe erythema with or without edema

Method remarks:

At the start of the induction phase, the body weight range of the test and primary challenge animals ranged from 336-493 g; animals were the same age (± 5 days) and were 6-11 weeks old. At the start of the rechallenge phase, the body weights of the rechallenge animals ranged from 426-599 g.

HISTORICAL POSITIVE CONTROL GROUP: 10 animals received 3 induction treatments with α-hexylcinnamaldehyde (HC) (tech., 85%) at concentrations of 5% w/v in 95% ethanol. Approx. 2 wks following induction, a primary challenge treatment was conducted with the 10 test animals and 4 naïve control animals with HC at 5%, 2.5%, and 1.0% w/v in acetone. 13 days following primary challenge treatment, a rechallenge treatment was conducted with the 10 test animals and 5 naïve control animals with HC at 5% w/v in acetone.

PILOT (IRRITATION SCREENING): The irritation potential of the test material at levels of undiluted, 50%, 25%, 10%, 5%, 2.5%, 1%, and 0.5% were evaluated. The position of the different concentrations on the animals were varied to adjust for possible site-to-site variation in response. One day prior to exposure, hair was removed from backs with clippers. 0.3 ml test preparation was applied to a 25 mm Hill Top Chamber®. The animal was placed into a restrainer, the chamber was applied to the clipped surface, and the chamber was occluded with rubber dental dam. Approximately 6 hr later, the chamber and restrainer were removed.

INDUCTION: An undiluted concentration of C16/C18 Alpha Olefins, Isomerized in Mineral Oil, was chosen for induction. The left shoulders of 20 animals were clipped the day before exposure. The clipped areas were exposed and animals restrained as described for the Pilot. The

procedure was repeated at the same site once a week for 2 wks. After the last induction exposure, the animals were left untreated for 12 days.

PRIMARY CHALLENGE: Using the same procedure as in the induction phase but at a different skin site, the test animals (10 M, 9 F) were again exposed to the test material (5% in Mineral Oil). In addition, 10 naïve animals were treated with the test material.

RECHALLENGE: 7 days after primary challenge, test animals (10 M, 9 F) were again exposed to the test material (5% in Mineral Oil). In addition, 10 naïve animals were treated with the test material.

OBSERVATIONS: On the day following irritation screening, primary challenge, and rechallenge, animals were depilated and, 2 hr later, scored. Scoring was repeated the following day. No statistical analysis was conducted.

Results: Animals treated with C16/C18 Alpha Olefin, Isomerized were not sensitized

Grades: The incidence of grade 1 responses in the test group (12/19) compared to that of the naïve control group (4/10) suggested the possibility that sensitization might have been induced. Following rechallenge, the incidence of grade 1 responses in the test group (12/19) compared to that of the naïve control group (8/10) indicated that sensitization had not been induced.

Results Remarks: One female was found dead 3 days after first induction application. Cause of death was not determined.

Reliability: (1) Reliable without restrictions

Reference: Morris, T. (1995) Delayed contact hypersensitivity study in guinea pigs (Buehler technique). Conducted by Hill Top Biolabs, Inc., Project No. 94-8414-21, for Chevron Research and Technology Company (unpublished report).

D. Test Substance: CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only)
(<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method: Magnusson and Kligman
Test Type: challenge
GLP: No
Year: 1997

Test Conditions

Species:	Guinea pig
Strain:	Dunkin-Hartley strain
Sex:	Female
Number of animals per sex per dose:	20 in test group; 10 in control group
Route of administration:	Injection and Topical
Intradermal	
Induction conc.:	25% w/v
Induction vehicle:	arachis oil
Induction conc.:	25% w/v in a mixture of Freund's Complete Adjuvant plus distilled water (1:1)
Induction vehicle:	arachis oil
Topical	
Induction conc.:	undiluted
Induction vehicle:	none
Challenge conc.:	75% and 50%
Challenge vehicle:	arachis oil

Method remarks:

A preliminary screen was carried out using groups of 4 guinea pigs to determine the concentrations of test material to be used for intradermal induction, topical induction and topical challenge. INTRADERMAL INDUCTION: The animals were injected intradermally with 1%, 5%, 10%, or 25% w/v in arachis oil. The injection sites were assessed aproximately 24, 48 and 72 hrs and 7 days after injection. The highest concentration that caused only mild to moderate skin irritation and was well tolerated systemically was selected for the intradermal induction stage. TOPICAL INDUCTION: Two guinea pigs (intradermally injected with Freunds's complete Adjuvant 21 days earlier) were treated with undiluted test material and 3 preparations of the test material (75%, 50% and 25% v/v in arachis oil). The highest concentration that caused only mild to moderate skin irritation after a 48-hr occlusive exposure was selected for the topical induction stage. TOPICAL CHALLENGE: Undiluted test material and 3 preparations of the test material (75%, 50% and 25% v/v in arachis oil) were applied occlusively to the flanks of 2 guinea pigs for a period of 24 hrs. The highest non-irritant concentration and one lower concentration were selected for the topical challenge stage of the main study.

Induction was accomplished in 2 stages, intradermal injection and a topical application. Immediately before treatment the hair was removed from an area approximately 40 mm x 60 mm on the shoulder region of each animal. A row of 3 injections (0.1 mL) was made on each side of the mid-line: Freund's complete adjuvant (FCA) and distilled water (1:1), a 25% w/v formulation of test material in arachis oil, and a 25% w/v formulatioin of test material in a 1:1 preparation of FCA plus distilled water. Approximately 24 and 48 hrs after intradermal injection, the degree of erythema was evaluated.

One week after the intradermal injections, the same area was clipped. A 4x4 cm patch of Whatman No. 3 filter paper was soaked in a solution of the test material, placed over the injection sites of the experimental animals and covered by overlapping plastic adhesive tape (Blendaderm) and secured with aluminium foil. This was secured with elastic adhesive bandage (Elastoplast). The occlusive dressing was left in place for 48 hours.

The challenge procedure was carried out on Day 21. Challenge was accomplished by topical application of the challenge solution of the test material to the flank of both test and control groups of animals. A 50x70 mm area on the flank was clipped and shaved. A 20x20 mm patch of Whatman No. 4 filter paper was soaked in a solution of the test material, placed over the injection sites on the right shoulder of the experimental animals and covered by overlapping plastic adhesive tape (Blendaderm). To ensure that the maximum non-irritant concentration was used at challenge, the test material at a concentration of 50% v/v in arachis oil was also similarly applied to a separate skin site on the left shorn flank. The patches were occluded with aluminium foil and secured with elastic adhesive bandage (Elastoplast). The dressing was left in place for 24 hours. Shortly before the 24-hr observation, the flanks were clipped. Examination of the challenge site was 24 and 48 hours after removal of the dressing.

Results: Negative for sensitization

Results Remarks: Number of animals with skin reaction at challenge: 0/20
Number of animals with skin reaction in control group at challenge: 0/10.

Reliability: (1) Reliable without restrictions

Reference: Driscoll, R. (1998) Magnusson & Kligman Maximisation Study in the Guinea Pig with C20-C24 Alkenes, Branched and Linear, Report 703/120. Conducted by Safepharm Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

E. **Test Substance:** CAS No. 93924-10-8, C20-24 Alpha Olefin

Method: Buehler, 1965; Ritz and Buehler, 1980

Test Type: challenge
GLP: Yes
Year: 1992

Test Conditions

Species: Guinea pig
Strain: No data

Sex:	No data
Number of animals per sex per dose:	20 test and 10 control, sex unknown
Route of administration:	Topical
Induction conc.:	undiluted
Induction vehicle:	None
Challenge conc.:	5%
Challenge vehicle:	Light mineral oil
Grading system used:	Buehler

Results: Negative for sensitization

Reliability: (1) Reliable without restrictions

Reference: Shell Oil Company (1992) Delayed contact hypersensitivity study in guinea pigs (Buehler technique): Neodene 20-24 alpha olefin. Ref 91-8384-21(B) (unpublished report).

Buehler, E.V. (1965) Delayed contact hypersensitivity in the guinea pig, *Archives of Dermatology* 91:171-177.

Ritz, H.L. and E.V. Buehler (1980) Planning, conduct and interpretation of guinea pig sensitization patch tests in *Current Concepts in Cutaneous Toxicity*, ed. V. Drill and P. Lazar. Academic Press, New York, N.Y. pp. 25-42.

5.5 Repeated Dose Toxicity

A. Test Substance

Identity (purity):	C16/18 isomerised olefin
Remarks:	C14-0.4%, C16-53.6%, C18-37.6%, C20-7.9%, C22-0.5%. Linear terminal 1.8%, linear internal 71.9%, Branched terminal 15.6% Trisubstituted 10.7%.

Method

Method/guideline:	OECD 407
Test type:	subacute toxicity
GLP:	Yes
Year:	2000
Species:	Rat
Strain:	Sprague Dawley (crl:CD BR)
Route of Administration:	Oral gavage
Duration of test:	4 weeks
Doses:	0, 25, 150, or 1000 mg/kg./day
Sex:	Males and females

Exposure period:	4 weeks
Frequency of treatment:	Once daily, 7 days/week
Control group and treatment:	Concurrent vehicle control (corn oil)
Post exposure observation period:	None
Statistical methods:	Analysis of variance (Snedecor and Cochran, 1980) Kruskal-Wallis non-parametric analysis (Hollander and Wolfe, 1973) Fisher's Exact Probability test (Siegel 1956)
Test Conditions:	Groups of ten rats (5M:5F) were dosed orally by gavage once daily over a period of 28 days. Animals were approximately 41 days old on the first day of dosing. Animals were regularly monitored for any signs of ill health or reaction to treatment. Detailed functional observations were performed weekly, with additional functional observations performed during pretrial and week four. Body weights and food consumption were recorded twice weekly. Blood and urine samples were collected during week four of the study. After four weeks of treatment animals were sacrificed and subjected to necropsy. A comprehensive list of organs were weighed and /or preserved preserved (adrenal, brain, epididymis, eye, gastrointestinal tract including stomach, duodenum, jejunum, ileum, caecum, colon, rectum, heart, kidney, liver, lung, bone marrow, mesenteric lymph node, ovary, pituitary, prostate, sciatic nerve, spinal cord, spleen, submandibular lymph node, testis, thymus, thyroid with parathyroid, trachea, urinary bladder, uterus). Tissues from the controls and high dose animals were subjected to histological examination. Histology was also performed on the male kidneys from the lower doses.
Results	
NOAEL (NOEL):	NOAEL = 1000 mg/kg/day
Actual dose received by dose level by sex if known:	Actual doses for both sexes were 0, 25, 150, or 1000 mg/kg/day.
Remarks:	There was little evidence of toxicity noted in animals treated at levels up to 1000 mg/kg/day. A slight increase in male body weight was noted at 1000 mg/kg but did not achieve statistical significance. Statistically significant, but equivocal, changes in urinary volume (higher than controls) and kidney weight (lower than controls) were considered unlikely to be treatment related in the absence of any macro- or microscopic changes. There were no treatment related findings associated with treatment at 25 or 150 mg/kg/day.
Reliability:	(1) Reliable without restrictions.
Flag:	Key study for SIDS endpoint.

References: Clubb, S. (2000) AmoDrill 1000 4-Week Toxicity Study Including Neurotoxicity Screening in Rats with Administration by Gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE Scotland. Sponsor Amoco Corporation (unpublished report).

B. Test Substance

Identity (purity): CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 408
Test type:	Subchronic Oral Toxicity - Rodent: 90-day Study
GLP:	Yes
Year:	1999
Species:	Rat
Strain:	Crl:CD BR
Route of Administration:	Oral gavage
Duration of test:	17 weeks
Doses:	0, 100, 500, and 1000 mg/kg /day
Sex:	Males and females
Exposure period:	13 weeks
Frequency of treatment:	Once daily
Control group and treatment:	Concurrent vehicle control (corn oil)
Post exposure observation period:	4 weeks

Statistical methods: All statistical analyses were carried out separately for males and females. If the data consisted predominantly of one particular value (relative frequency of the mode exceeded 75%), the proportion of animals with values different from the mode was analyzed (Fisher, 1950; Mantel, 1963). Otherwise, a test was applied to test for heterogeneity of variance between treatments (Bartlett, 1937). Where significant (at the 1% level) heterogeneity was found, a logarithmic transformation was tried to see if a more stable variance structure could be obtained. Except for predose data, analyses of variance were followed by Student's t test and Williams test (Williams, 1971, 1972) for a dose related response, although only the one thought most appropriate for the response pattern observed was reported. The Kruskal-Wallis analyses were followed by the non-parametric equivalents of these tests (Shirley, 1977). When appropriate,

analysis of covariance was used in place of analysis of variance in the above sequence. For most parameters, the appropriate covariance was the same parameter at predose. For organ weight data, analysis of variance was performed using terminal bodyweight as covariate when the within group relationship between organ weight and bodyweight was significant at the 10% level.

Test Conditions:

In a preliminary range-finder study, test material was administered by gavage to a group of 3 male and 3 female Sprague-Dawley CD strain rats for twenty-eight consecutive days at a dose level of 1000 mg/kg/day. A control group of 3 males and 3 females remained untreated throughout the study period but was otherwise handled in an identical manner to that of the test animals.

In the 13-week study with 28-day recovery period, animals were 6 wks old at the start of treatment and weighed 146-189 g (males) and 131-169 g (females). The test material was administered by gavage to groups of 20 male and 20 female Sprague-Dawley CD strain rats at 1000 mg/kg/day and 10 animals of each sex at 100 and 500 mg/kg/day for a period of 13 weeks. A control group of 20 males and 20 females received the vehicle, corn oil. At the end of the 13-week treatment period 10 males and 10 females from each group were sacrificed; the remaining 10 male and 10 female animals from the control and high dose groups were maintained, undosed for a 4-week period to assess recovery. Clinical signs, bodyweight, and food and water consumption were monitored during the study, and ophthalmoscopy and neurobehavioral screening (motor activity and functional observational battery) were performed. On completion of 13 weeks of treatment and/or 4 weeks of recovery, all surviving animals were killed and a full macroscopic examination of the tissues was performed. All superficial tissues, the abdominal viscera, the gastrointestinal tract and organs including adrenals, lungs, kidneys, liver, gonads, uterus, intra-abdominal lymph nodes and accessory reproductive organs were examined visually and by palpation. The following organs were dissected free of fat and weighed: adrenals, brain, epididymides, heart, kidneys, liver, ovaries, pituitary, spleen, testes, thymus, thyroid (with parathyroids) and uterus (with cervix). Samples of all the tissues were preserved in buffered 10% formalin (except eyes, which were preserved in Davidson's fixative, and testes and epididymides which were initially placed in Bouins solution and transferred to 70% alcohol). Tissues required for microscopic examination in the study (adrenals, alimentary tract, brain, epididymides, eyes, femur, heart, kidneys, liver, lungs, lymph nodes, mammary gland, ovaries, pancreas, pituitary, prostate, salivary glands, sciatic nerve, seminal vesicles, skeletal muscle, spinal column, spleen, sternum, testes, thymus, thyroids, trachea, urinary bladder and uterus) were embedded in paraffin wax and sections cut at 4 micrometers were stained with haematoxylin and eosin. Tissues of testes were stained using a standard PAS method.

The dosing solutions were analyzed for stability, homogeneity and concentration. Prior to treatment, the homogeneity and stability for the

dosing formulation was confirmed at nominal concentrations of 1 mg/ml and 200 mg/ml during ambient temperature storage for 2 days and refrigerated storage for 15 days, a period representing the maximum time from preparation to completion of dosing. Formulations used during the study were analyzed for concentration.

Results

NOAEL (NOEL): NOAEL = 1000 mg/kg/day
NOEL = 100 mg/kg/day (males - glucose); 500 mg/kg/day for females (liver weight and adrenal hypertrophy)

LOAEL (LOEL): LOEL = 500 mg/kg/day (males); 1000 (females)

Actual dose received by dose level by sex if known: The mean concentration of C20-24 alkenes, branched and linear, in test formulations analyzed during the study were within ± 12% of nominal concentrations, confirming the accuracy of formulation.

Remarks: In a preliminary rangefinder study, no treatment-related changes in the parameters measured were found. The "No Observed Effect Level" (NOEL) is therefore considered to be 1000 mg/kg/day.

In the 13-wk study, there were no deaths during the study. No clinical signs or effects on bodyweight or food intake were seen. No ophthalmological or neurobehavioral effects were noted. Slight, statistically significant, yet reversible changes in haematological parameters were noted amongst animals receiving 1000 mg/kg/day when compared with the controls: lower packed cell volume of males and females, lower haemoglobin levels of males, lower erythrocyte count of females and longer clotting times of males at the end of the 13-week treatment. Group mean glucose levels were statistically significantly higher amongst male rats receiving 500 and 1000 mg/kg/day in the 13 week study when compared with controls. These effects were not apparent at the end of the 4-week recovery period. In the absence of any obvious dose response or any consistency across the sexes, these effects were considered to be of no toxicological importance.

Minimal, adaptive hepatic changes (centrilobular hepatocyte hypertrophy) associated with statistically significant higher group mean liver weight (12.5, 13.2, 14.4, 13.9 g for control, 100, 500, 1000 mg/kg/day, respectively), were detected in a small number of females of all treated groups (1 for 100 mg/kg/day, 3 for 500 mg/kg/day, and 4 for 1000 mg/kg/day), but not in any control females. The increased incidence was statistically significant only among females of the 1000 mg/kg/day group. A statistically significant increased incidence of minimal or slight adrenal cortical hypertrophy was noted amongst females receiving 1000 mg/kg/day compared with controls (2 for control, 2 for 100 mg/kg/day, 3 for 500 mg/kg/day, and 10 for 1000 mg/kg/day) associated with increased adrenal weight (71.6, 72.9, 87.2, 84.8 g for control, 100, 500, 1000 mg/kg/day, respectively). A significantly

increased incidence of minimal or slight epithelial hyperplasia in the stomach was noted amongst males receiving 1000 mg/kg/day (7 incidences, controls: 2 incidences), which could be associated with the route of administration. These findings were not present following a 4-week recovery period. The study report author assigned a NOAEL of 1000 mg/kg/day.

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint.

References: Brooker AJ (1999). C20-24 Alkenes, branched and linear: Toxicity Study By Oral Gavage Administration to CD Rats for 13 Weeks Followed by a 4-Week Recovery Period. Project Nos. CHR/052 and CHR/053. Conducted by Huntingdon Life Sciences for Chevron Research and Technology Company (unpublished report).

C. Test Substance

Identity (purity): CAS 27070-58-2, Octadecenes; CAS 182636-02-8, Branched Octadecenes

Remarks: Test substance identified as Octadecene C18 Compound; 96.7% C18 olefins; 1.84% C16 olefins, 0.95% C20 olefins; 3.30% normal alpha olefins; 32.5% methyl branched isomers; 67.5% linear olefins.

Method/guideline:	OECD 421 (see Sections 5.9.A(1) and 5.9.B for reproductive toxicity endpoints)
Type:	Reproduction/Developmental Toxicity Screening Test
GLP:	Yes
Year:	2003
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Oral gavage
Concentration levels:	0, 100, 500 and 1000 mg/kg/day
Sex:	Male and female
Control group and treatment:	Corn oil by oral gavage (5 mL/kg)
Frequency of treatment:	Daily
Duration of test:	Through lactation day 4 for pups
Premating exposure period for males:	Two weeks
Premating exposure period for females:	Two weeks
Statistical methods:	See Section 5.9.A.(1)

Test Conditions: See Section 5.9.A(1). General toxicity endpoints were limited to mortality, clinical observations, bodyweight, food consumption, gross necropsy examination, and reproductive organ weights and histopathology. Treatment was for approximately 56 days.

Results

NOAEL:	NOAEL for general toxicity = 1000 mg/kg/day (limited endpoints)
Actual dose received by dose level by sex if known:	All dosing formulations were found to be within 20% of the stated concentration.
Maternal and Paternal general toxicity:	No toxicologically meaningful effects seen at 1000 mg/kg/day (see Section 5.9.A(1) for details)
Reliability:	(1) Reliable without restrictions
References:	Thorsrud, B.A. (2003) An oral (gavage) reproduction/developmental toxicity screening study in Sprague Dawley rats with (C18) Octadecenes. Report No. 3604.1. Conducted by Springborn Laboratories, Spencerville, OH, for American Chemistry Council Higher Olefins Panel (unpublished study).

5.6 Genetic Toxicity *in vitro*

A. Gene Mutation

(1) Test Substance

Identity (*purity*):	CAS No. 112-88-9, 1-Octadecene (SHOP C18 linear alpha olefin)
Remarks:	Source: S.O.C., Houston, Texas. Stability during use confirmed by an NMR technique.

Method

Method/guideline:	Similar to OECD 471
Type:	in-vitro bacterial reverse mutation – Ames Assay
System of testing:	bacterial
GLP:	No
Year:	1980
Species/Strain:	Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100. Escherichia coli strains WP_2 and WP_2 uvrA.
Metabolic activation:	With and without S9 fraction from Arochlor induced rat liver
Concentrations tested:	0, 0.2, 2.0, 20, 200, and 2000 µg/plate

Statistical Methods:	Reproducible values of 2.5 X control value or greater are considered to indicate a mutagenic response.
Test Conditions:	Number of replicates: 3 per concentration; Solvent: acetone Temperature: 37°C for 48 hours; Positive control materials: 20 µg/plate of 4-nitroquinoline-N-oxide, sodium azide, or benzo(a)pyrene. Experiments were carried out in duplicate.

Results

Cytotoxic conc.:	Concentrations used were not reported as cytotoxic
Genotoxic effects:	Negative with and without metabolic activation
Remarks:	The addition of Alpha C18 Product to agar layer cultures of the bacterial tester strains, with or without the incorporation of rat liver microsomal fraction, did not result in an increase in the reversion frequency in any of the strains. All positive and negative controls responded in a manner consistent with data from previous assays.
Reliability:	(2) Reliable with restrictions: comparable to guideline study with acceptable restrictions
Flag:	Key study for SIDS endpoint.
References:	Dean BJ. Shell Chemicals Europe Ltd. (1980) Toxicity Studies with Detergent Intermediates: In Vitro Genotoxicity Studies with SHOP Process Intermediates. Shell Toxicology Laboratory (Tunstall). Shell Report # TLGR.80.074 (unpublished report).

(2) Test Substance

Identity (*purity*):	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 471
Type:	in-vitro bacterial reverse mutation – Ames Assay
System of testing:	bacterial
GLP:	yes
Year:	1998
Species/Strain:	Salmonella typhimurium strains TA 1535, TA 1537, TA 98, and TA 100. Escherichia coli strain WP_2 uvrA.
Metabolic activation:	With and without S9 fraction from livers from rats induced with Arochlor 1254 (0.5 ml of 10% S9 mix per plate)

Concentrations tested: 0, 15, 50, 150, 500, 1500, 5000 μg/plate

Statistical Methods: For a substance to be considered positive in this test system, it should have induced a dose-related and statistically significant increase in the revertant count in one or more strains of bacteria in the presence and/or absence of S9 in both experiments. To be considered negative, the number of revertants at each dose level should have been less than twofold the vehicle control frequency for TA100, TA98 and WP2uvrA- and threefold for TA1535 and TA1537. Statistical significance was analyzed using the methods recommended by the UKEMS [Reference: Kirkland, D.J., Ed., Statistical Evaluation of Mutagenicity Test Data, UKEMS sub-committee on Guidelines for Mutagenicity Testing. Report Part III (1989) Cambridge University Press.].

Test Conditions: Bacterial strains were treated with the test material using the Ames plate incorporation method at six dose levels, in triplicate, both with and without the addition of a rat liver homogenate metabolizing system. The dose range was determined in a preliminary toxicity assay and was 15 to 5000 ug/plate in the first experiment. A second experiment was performed on a separate day using the same dose range as Experiment 1, fresh cultures of the bacterial strains, and fresh chemical formulations. Vehicle (acetone), untreated (negative) and positive controls were included in each experiment.

For the test, 0.1 mL of bacterial culture, 2.0 mL of top agar, 0.1 mL of the test material formulation, vehicle or positive control and either 0.5 mL of S9 mix or phosphate buffer was mixed together and poured onto the surface of a Vogel-Bonner Minimal agar plate. The plates were incubated for 48 hours at 37°C after an initial overnight equilibration period and the frequency of revertant colonies was assessed.

Results

Cytotoxic conc.: None
Genotoxic effects: Negative with and without metabolic activation

Remarks: The test material caused no visible reduction in the growth of the bacterial lawn at any dose level either with or without metabolic activation. The test material was therefore tested up to a maximum recommended dose level of 5000 ug/plate. A precipitate was observed at and above 1500 ug/plate; this however did not interfere with the scoring of revertant colonies. No significant increase in the frequency of revertant colonies was recorded for any of the bacterial strains with any dose of the test material, either with or without metabolic activation.

The vehicle (acetone) and untreated control plates produced

counts of revertant colonies within the normal range.

All of the positive control chemicals used in the test induced marked increases in the frequency of revertant colonies and the activity of the S9 fraction was shown to be satisfactory.

The test material was found to be nonmutagenic under the conditions of this test.

Reliability: (1) Reliable without restrictions

References: Thompson PW (1998) C20-24 Alkenes, Branched and Linear: Salmonella typhimurium and Escherichia coli/Mammalian-Microsome Reverse Mutation Assay, SafePharm Laboratories Limited Project No. 703/086. Conducted for Chevron Research and Technology Company (unpublished report).

(3) Test Substance

Identity: CAS Nos. C24=182636-05-1, C26=182636-06-2, C28=182636-07-3, C30=182636-08-4: C24-30 Alkenes, Branched and Linear

Remarks: even-numbered carbons only (<55% C24, <40% C26, <15% C28, <30% C30; 70%branched)

Method

Method/guideline: OECD 471
Type: in-vitro bacterial reverse mutation – Ames Assay
System of testing: bacterial
GLP: yes
Year: 2000
Species/Strain: Salmonella typhimurium strains TA 1535, TA 1537, TA 98, and TA 100. Escherichia coli strain WP_2 uvrA.

Metabolic activation: With and without S9 fraction from livers from rats induced with Arochlor 1254 (0.5 ml of 10% S9 mix per plate)

Concentrations tested: 0, 15, 50, 150, 500, 1500, 5000 µg/plate

Statistical Methods: For a substance to be considered positive in this test system, it should have induced a dose-related and statistically significant increase in the revertant count in one or more strains of bacteria in the presence and/or absence of S9 in both experiments. To be considered negative, the number of revertants at each dose level should have been less than twofold the vehicle control frequency for TA100, TA98 and WP2uvrA- and threefold for TA1535 and TA1537. Statistical significance was analyzed using the methods recommended by the UKEMS [Reference: Kirkland, D.J., Ed., Statistical Evaluation of Mutagenicity Test Data, UKEMS sub-

committee on Guidelines for Mutagenicity Testing. Report Part III (1989) Cambridge University Press.].

Test Conditions: Bacterial strains were treated with the test material using the Ames plate incorporation method at six dose levels, in triplicate, both with and without the addition of a rat liver homogenate metabolizing system. The dose range was determined in a preliminary toxicity assay and was 15 to 5000 ug/plate in the first experiment. A second experiment was performed using the same dose range as Experiment 1, fresh cultures of the bacterial strains, and fresh chemical formulations. Vehicle, dimethyl sulphoxide (DMSO), untreated (negative) and positive controls were included in each experiment.

For the test, 0.1 mL of bacterial culture, 2.0 mL of top agar, 0.1 mL of the test material formulation, vehicle or positive control and either 0.5 mL of S9 mix or phosphate buffer was mixed together and poured onto the surface of a Vogel-Bonner Minimal agar plate. The plates were incubated for 48 hours at 37oC after an initial overnight equilibration period and the frequency of revertant colonies was assessed.

Results

Cytotoxic conc.: None
Genotoxic effects: Negative with and without metabolic activation

Remarks: The test material caused no visible reduction in the growth of the bacterial lawn at any dose level either with or without metabolic activation. The test material was therefore tested up to a maximum recommended dose level of 5000 ug/plate. An opaque film was observed at and above 1500 ug/plate with oily droplets observed at 5000 ug/plate under a dissection microscope; this however did not interfere with the scoring of revertant colonies. No significant increase in the frequency of revertant colonies was recorded for any of the bacterial strains with any dose of the test material, either with or without metabolic activation.

The vehicle, dimethyl sulphoxide (DMSO) and untreated control plates produced counts of revertant colonies within the normal range.

All of the positive control chemicals used in the test induced marked increases in the frequency of revertant colonies and the activity of the S9 fraction was shown to be satisfactory.

The test material was found to be nonmutagenic under the conditions of this test.

Reliability: (1) Reliable without restrictions

References: Thompson PW (1998) C24-30 Alkenes, Branched and Linear: Salmonella typhimurium and Escherichia coli/Mammalian-Microsome Reverse Mutation Assay, SafePharm Laboratories Limited Project No. 703/087. Conducted for Chevron Research and Technology Company (unpublished report).

B. Chromosomal Aberration

(1) Test Substance

Identity (*purity*): CAS No. 112-88-9, 1-Octadecene (SHOP C18 linear alpha olefin)

Remarks: Source: S.O.C., Houston, Texas. Stability during use confirmed by an NMR technique.

Method

Method/guideline:	Not specified
Type:	In-vitro mammalian cell chromosome aberration test
System of testing:	non- bacterial
GLP:	No
Year:	1980
Cell line:	Rat liver (RL_1) cells
Metabolic activation:	None
Concentrations tested:	0, 125, 250, 500 µg/ml as an acetone solution
Statistical Methods:	No specifics noted. Positive responses indicated as higher frequency of chromosome damage as was seen with the positive control substance

Test Conditions: Number of replicates: 3 per concentration. Frequency of Dosing: continuous. Solvent: acetone. Positive control: dimethylbenzanthracene (1.0µg/ml). RL_1 slide cultures were exposed to culture medium containing the test materials at final concentrations equivalent to 0.5x, 0.25x, and 0.125x the concentration inhibiting cell proliferation by 50 % (GI_{50} concentration). After 24 h the cultures were processed for chromosome analysis and where possible 100 cells were analyzed from each of three cultures per dose group. A repeat assay was performed in order to verify the data produced in the initial assay. The range of concentrations of the test compound to be used to assess the cloning efficiency was determined from the results of the initial assay. For each concentration, including the solvent control, three 9 cm diameter Petri dishes were used. Five hundred RL4 cells were added to each dish and cells were incubated in 10 ml tissue culture medium at 37°C in a humidified atmosphere containing 5% CO2. Twenty-four hours after adding the cells, the medium was replaced with medium containing the

compound or solvent, which was replaced with fresh medium after 24 hours exposure. Five days later, the cells were fixed and stained. Colonies containing at least 50 cells were counted. The SBGR concentration of the test compound that reduced the number of colonies to an average of approximately 50% of those on the dishes exposed to solvent only was used as the highest concentration in the chromosome assay.

Results

Cytotoxic conc.: Concentrations used were not reported as cytotoxic

Genotoxic effects: Negative

Remarks: The concentration range of C18 product that it was possible to test was restricted since the compound was insoluble in DMSO. However, reasonably high concentrations of the compound (500 mg/ml) were soluble in acetone. In preliminary cytotoxicity studies, no toxic effects were observed in RL_1 cells up to a concentration of 500 µg/ml. Therefore 500 µg/ml alpha C18 product was used as the highest dose in the subsequent chromosome assay. A single exchange figure was observed on one culture treated with 250 µg/ml alpha C18 product. However, since no dose related increase in the frequency of chromatid gaps, chromatid breaks or total chromatid aberrations was observed, it was concluded that alpha C18 product did not induce a cytogenetic effect in cultured RL_1 cells.

Reliability: (2) Reliable with restrictions: comparable to guideline study with acceptable restrictions

Flag: Key study for SIDS endpoint

References: Dean BJ. Shell Chemicals Europe Ltd. (1980). Toxicity Studies with Detergent Intermediates: In Vitro Genotoxicity Studies with SHOP Process Intermediates. Shell Toxicology Laboratory (Tunstall). Shell Report # TLGR.80.074 (unpublished report).

(2) Test Substance

Identity (*purity*): CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only)
(<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline: OECD 473

Type:	In-vitro mammalian cell chromosome aberration test
System of testing:	non- bacterial
GLP:	Yes
Year:	1998
Cell line:	Cultured human lymphocytes
Metabolic activation:	With and without S9 fraction from Aroclor 1254 induced rats
Concentrations tested:	39.06 – 5000 µg/mL
Statistical Methods:	Fisher's Exact test

Test Conditions: Human lymphocytes treated with the test material were evaluated for chromosome aberrations at five dose levels, in duplicate, together with vehicle (acetone) and positive controls. In experiment 1, cells were exposed for 4 hours, with and without the addition of an induced rat liver homogenate metabolizing system (S9 at 10% in standard co-factors, final concentration 1%), harvested 20 hours after treatment initiation. Results were confirmed in a second experiment with a 4-hour exposure with metabolic activation (at 20% in standard co-factors, final concentration 2%) and a 20-hour continuous exposure in the absence of activation, and harvest at 20 hours after treatment initiation. The dose levels selected for evaluation for chromosome aberrations (312.5, 625, 1250, 2500, and 5000 µg/ml) were selected on the basis of toxicity demonstrated by the mitotic index. Slides were coded and blindly scored. A total of 2000 lymphocyte cell nuclei were counted and the number of cells in metaphase recorded and expressed as the mitotic index and as a percentage of the vehicle control value. Where possible, the first 100 consecutive well-spread metaphases from each culture were counted, and if the cell had 44 or more chromosomes, any gaps, breaks or rearrangements were noted. The frequency of cells with aberrations (both including and excluding gaps) and the frequency of polyploid cells were compared, where necessary, with the concurrent vehicle control value using Fisher's Exact test.

Results

Cytotoxic conc.:	> 5000 µg/mL
Genotoxic effects:	Negative with and without metabolic activation.
Remarks:	An oily layer on the surface of the media was observed at and above 312.5 ug/ml when dosed into media. Presence of an oily precipitate was also observed after spinning at both the washing and harvesting stage. There was no mitotic inhibition at any dose level assessed either in the absence or presence of S9. All vehicle (solvent) controls gave frequencies of cells with aberrations within expected ranges.

All positive control treatments gave statistically significant increases in the frequency of cells with aberrations indicating the satisfactory performance of the test and the activity of the metabolising system.

The test material did not induce any statistically significant increases in the frequency of cells with chromosome aberrations or numbers of polyploid cells.

The test material was shown to be non-clastogenic to human lymphocytes in vitro.

Reliability: (1) Reliable without restrictions

References: Wright NP (1998) C20-24 Alkenes, Branched and Linear: Chromosome Aberration Test in Human Lymphocytes In Vitro, SafePharm Laboratories Limited Project No. 703/122. Conducted for Chevron Research and Technology Company (unpublished report).

C. Other Genetic Effects

Test Substance

Identity (*purity*): CAS No. 112-88-9, 1-Octadecene (SHOP C18 linear alpha olefin)

Remarks: Source: S.O.C., Houston, Texas. Stability during use confirmed by an NMR technique.

Method

Method/guideline: Similar to OECD 481
Type: Mitotic Gene Conversion
System of testing: non-bacterial
GLP: No
Year: 1980
Species/Strain: Saccharomyces cerevisiae JD1
Metabolic activation: With and without S9 fraction from Arochlor induced rat liver
Concentrations tested: 0, 0.01, 0.1, 0.5, 1.0 and 5.0 mg/ml
Statistical Methods: Reproducible values of greater than twice the control value are considered to indicate a mutagenic response.

Test Conditions: Number of replicates: 3 per concentration; Solvent: acetone; Positive control materials: cyclophosphamide (10 mg/ml) or 4-nitroquinoline-N-oxide (0.001 or 0.0001 mg/ml). Liquid suspension cultures of Saccharomyces cerevisiae JD1 were dosed with 20 µl (without S9 mix) or 25 µl (with S9 mix) of appropriate solutions or suspensions of Alpha C18 Product to give final concentrations of 0.01, 0.1, 0.5, 1.0, and 5.0 mg/ml. Three replicate experiments were carried out and incubation periods of 1 h at room temperature for experiments without S9 and 1 or 4 h at 37°C in a shaking water bath in the presence of S9 were used.

The mitotic gene conversion was calculated from counts of revertant colonies after 3 days incubation of the plate cultures at 30°C.

Results

Cytotoxic conc.:	Concentrations used were not reported as cytotoxic
Genotoxic effects:	Negative with and without metabolic activation
Remarks:	The addition of Alpha C18 product to liquid suspension cultures of Saccharomyces cerevisiae JD1, with or without the incorporation of rat liver S9 fraction, did not induce a consistent increase in mitotic gene conversion at either gene locus in three replicate experiments.
Reliability:	(2) Reliable with restrictions: comparable to guideline study with acceptable restrictions
References:	Dean BJ. Shell Chemicals Europe Ltd. (1980) Toxicity Studies with Detergent Intermediates: In Vitro Genotoxicity Studies with SHOP Process Intermediates. Shell Toxicology Laboratory (Tunstall). Shell Report # TLGR.80.074 (unpublished report).

5.7 Genetic Toxicity *in vivo*

Test Substance

Identity (purity):	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only) (<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline:	OECD 474
Type:	Micronucleus Assay
GLP:	Yes
Year:	1998
Species:	Mouse
Strain:	CD-1
Sex:	Male
Route of Administration:	i.p.
Concentration levels:	500, 1000 and 2000 mg/kg
Exposure period:	24 and 48 hrs
Statistical methods:	A positive mutagenic response was demonstrated when a statistically significant and dose responsive increase in the number of micronucleated polychromatic erythrocytes was observed for either the 24 or 48-hour kill times when compared to their corresponding control group. A positive response for bone marrow toxicity was demonstrated when the dose group mean polychromatic to normochromatic ratio was shown to be statistically significantly lower than that

of the concurrent vehicle control group. All data were statistically analysed using appropriate statistical methods as recommended by the UKEMS Sub-committee on Guidelines for Mutagenicity Testing Report, Part III (1989).

Test Conditions: A study was performed to assess the potential of the test material to produce damage to chromosomes or aneuploidy when administered via the intraperitoneal route to five to eight week old mice. Following a preliminary range-finding study in males and females which showed no adverse effects at 2000 mg/kg, the micronucleus study was conducted in males only, using the test material at the maximum recommended dose level of 2000 mg/kg with 1000 and 500 mg/kg as the lower two dose levels. In the micronucleus study, groups of seven male mice were given single intraperitoneal doses of the test material at 2000, 1000, and 500 mg/kg diluted with arachis oil. Further groups of mice were dosed via the intraperitoneal route with arachis oil (7 mice) or orally with cyclophosphamide (5 mice) to serve as vehicle and positive controls, respectively. Animals were killed 24 hours (all doses and controls) and 48 hours (high dose and control only) after exposure. The bone marrow was extracted from femurs, and smear preparations were made and stained. The incidence of micronucleated cells per 2000 polychromatic erythrocytes (PCE) per animal was scored. In addition, the number of normochromatic erythrocytes (NCE) associated with 1000 erythrocytes was counted; these cells were also scored for incidence of micronuclei.

Results

Effect on PCE/NCE ratio: None

Genotoxic effects: Negative

NOEL: 2000 mg/kg

Remarks: There were no premature deaths or clinical signs observed in any of the dose groups. There was no evidence of a significant increase in the incidence of micronucleated polychromatic erythrocytes in animals dosed with the test material when compared to the concurrent vehicle control groups. No statistically significant decreases in the PCE/NCE ratio were observed in the 24 or 48-hour test material dose groups when compared to their concurrent control groups.

The positive control material produced a marked increase in the frequency of micronucleated polychromatic erythrocytes.

The test material, C20-24 Alkenes, Branched and Linear, was considered to be non-genotoxic under the conditions of the test.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Durward R (1998) C20-24 Alkenes, Branched and Linear: Micronucleus Test in the Mouse, SafePharm Laboratories Limited Project No. 703-121. Conducted for Chevron Research and Technology Company (unpublished report).

5.8 Carcinogenicity

Test Substance: CAS No. 112-88-9, 1-Octadecene

Method

Species:	mouse
Strain:	Rockland
Sex:	No data
Route of Administration:	Dermal
Frequency of Treatment:	Treated on 3 alternate days
Doses:	0.2 ml undiluted test material was applied topically to the shorn dorsal skin of mice, 3 or 4 animals/treatment group and 25 untreated controls
Control Group:	Yes, concurrent, no treatment

Test Condition: Mice, aged 7-10 weeks, were treated with 1-octene, 1-decene,1-dodecene, 1-tetradecene, 1-hexadecene, or 1-octadecene. The study was concerned with the measurement of changes in the skin sterols cholesterol and D7 cholestanol for the early assessment of skin carcinogenesis. Hyperplasia was evaluated by weight of epidermis/square cm.

Additionally, the appearance of the sebaceous glands is described following topical administration of alkenes and other products including carcinogens. The hypothesis was that the D7-cholestenol, depletion of which appeared indicative of carcinogenic activity, was concentrated in the sebaceous glands.

Results: It was found that the alkenes tested produced hyperplasia with a parallel increase in epidermal cholesterol while D7 cholestanol remained uniform, a pattern seen with the tumour promoter croton oil. This is in contrast to known carcinogens where the increase in epidermal weight and cholesterol is usually accompanied by a decrease in D7 cholestanol. The maximum activity for the series of alkenes was at C14.

There was damage to the sebaceous glands with known carcinogens or croton oil, but not with octadecene. This suggests that the pattern of hyperplasia seen following topical application of alkenes is not indicative of skin carcinogenic activity.

References: Brooks, S.C. and C.A. Baumann (1956) Skin Sterols, X. Studies with certain hyperplasia-inducing hydrocarbons. Cancer Res, 16: 357-363.

Brooks, S.C., J. J. Lalich, and C.A. Baumann (1957) Skin Sterols, XII. Contrasting effects of certain mercaptans, amines, and related compounds on sterols and sebaceous glands. Cancer Research 17: 148-153.

5.9 Reproductive Toxicity (including Fertility and Developmental Toxicity).

A. Fertility

(1) Test Substance

Identity (purity):	CAS 27070-58-2, Octadecenes; CAS 182636-02-8, Branched Octadecenes
Remarks:	Test substance identified as Octadecene C18 Compound; 96.7% C18 olefins; 1.84% C16 olefins, 0.95% C20 olefins; 3.30% normal alpha olefins; 32.5% methyl branched isomers; 67.5% linear olefins.

Method

Method/guideline:	OECD 421 (see Section 5.9.B for developmental toxicity endpoints)
Type:	Reproduction/Developmental Toxicity Screening Test
GLP:	Yes
Year:	2003
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Oral gavage
Concentration levels:	0, 100, 500 and 1000 mg/kg/day
Sex:	Male and female
Control group and treatment:	Corn oil by oral gavage (5 mL/kg)
Frequency of treatment:	Daily
Duration of test:	Through lactation day 4 for pups
Premating exposure period for males:	Two weeks
Premating exposure period for females:	Two weeks
Statistical methods:	Data, including body weights, body weight changes, food consumption, implantation sites, corpora lutea, gestation length and mean live litter size, were analyzed by ANOVA. If significance was observed with ANOVA, control to treatment group comparisons were performed using Dunnett's test. Count data were analyzed using R x C Chi-Square test followed by Fisher's Exact Test for copulation and fertility indices, pup sex ratios, the number of live and dead pups per group (on lactation day 0) and pup survival (after lactation day 0). Absolute and relative organ weights were analyzed for homogeneity of variance using Bartlett's test. If significance was detected with Bartlett's test ($p<0.01$), multiple group comparisons proceeded

using the Kruskal-Wallis non-parametric ANOVA, followed by Dunn's test, when $p<0.05$. If significance was not detected with Bartlett's test, parametric procedures were used to analyze the data, i.e., ANOVA followed by Dunnett's test when $p<0.05$. All statistical analyses were performed using the SLI Alpha ReproTox computer system (version 1.5.3 or later). All analyses were two-tailed with a minimum significance level of 5% ($p<0.05$).

Test Conditions: On day –1, animals were 9 wks of age with body weights ranging from 311 to 394 g for males and 201 to 262 g for females. The study consisted of a vehicle control and three treatment groups, with 12 males and 12 females in each group. Octadecenes C18 Compound was dissolved in corn oil and administered at dosage levels of 100, 500 and 1000 mg/kg/day, once daily by oral gavage, to F0 parental animals. All doses were given at a constant volume of 5 mL/kg. Control animals were administered corn oil under the same experimental conditions at an equivalent dose volume. F0 males were treated for two weeks prior to mating, during mating and four weeks following mating. F0 females were treated for two weeks prior to mating, during mating, during gestation and following parturition. Males and females were dosed up to and including the day prior to scheduled euthanasia. Following a minimum of 2 wks of treatment, each female was cohabited with a single male randomly selected from the same treatment group (1:1 pairing). Evidence of mating was determined by the presence of a copulatory plug in the vagina or a sperm positive vaginal smear. On approximately gestation day 18, females with confirmed copulation were transferred to individual boxes containing nesting material. Females and offspring remained together until lactation day 4. Both F0 parental animals and F1 offspring were closely examined for indications of toxicity. Experimental endpoints included clinical observations (cage-side observations daily and detailed observations weekly; during gestation and lactation, detailed observations performed daily for F0 females), body weights (Males: weekly and on day of euthanasia. Females: weekly until evidence of mating observed, and on gestation days 0, 7, 14 and 20; following parturition, on lactation days 1 and 4), food consumption (same days as body weights except during cohabitation), mating, parturition, lactation and offspring growth and viability. All F0 and F1 animals were subjected to a gross necropsy examination at the time of death or euthanasia on lactation day 4. Uterine contents were examined and the number of implantation sites and number of corpora lutea were recorded. All abnormalities were recorded. Testes and epididymides were weighed. The following organs were preserved: gross lesions, ovaries, prostate, epididymides, testes, seminal vesicles, uterus, vagina. Ovaries, testes and epididymides from control and high-dose animals were examined for histopathology. F1 pups were examined for viability (daily on days 0-4), external examinations

(days 0 and 4), sex determinations (days 0 and 4), body weights (days 1 and 4).

Results

NOAEL: NOAEL Parental (reproductive toxicity) = 1000 mg/kg
NOAEL for F1 offspring = 1000 mg/kg/day

Actual dose received by dose level by sex if known: All dosing formulations were found to be within 20% of the stated concentration.

Remarks: All animals in the vehicle control, 100, 500 and 1000 mg/kg/day groups survived to scheduled euthanasia. Most of the clinical signs that were observed during the course of the study were generally unremarkable in both F0 males and females and did not appear to follow any dose response pattern. There were no statistically significant or toxicologically meaningful differences noted in F0 mean body weights, body weight change or food consumption between the vehicle control and test article-treated groups. The F0 female mating and fertility indices and mean gestation lengths were comparable between the vehicle control and test article-treated groups. The mean number of F0 implantation sites and corpora lutea, the mean number of F1 pups delivered, the live birth and viability indices, and the mean live pups per litter and pup sex ratio on lactation days 0 and 4 were comparable between the control and test article-treated groups. No remarkable internal gross necropsy findings were noted for F0 males or females in the vehicle control or test article-treated groups at scheduled euthanasia. There were no statistically significant or toxicologically meaningful differences in the absolute or relative testes or epididymides weights of F0 males in the test article-treated groups compared to controls. There were no test article-related microscopic lesions noted in the testes, epididymides or ovaries from the vehicle control and 1000 mg/kg/day groups. Based on the results of this study, a dosage level of 1000 mg/kg/day was considered a no-observed-adverse-effect level (NOAEL) for reproductive effects.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Thorsrud, B.A. (2003) An oral (gavage) reproduction/ developmental toxicity screening study in Sprague Dawley rats with (C18) Octadecenes. Report No. 3604.1. Conducted by Springborn Laboratories, Spencerville, OH, for American Chemistry Council Higher Olefins Panel (unpublished study).

(2) **Test Substance**

Identity (purity):	C16/18 isomerised olefin
Remarks:	C14-0.4%, C16-53.6%, C18-37.6%, C20-7.9%, C22-0.5%. Linear terminal 1.8%, linear internal 71.9%, Branched terminal 15.6% Trisubstituted 10.7%.

Method

Method/guideline:	OECD 407 (see Section 5.5A for general toxicity endpoints)
Test type:	Subacute toxicity
GLP:	Yes
Year:	2000
Species:	Rat
Strain:	Sprague Dawley (crl:CD BR)
Route of Administration:	Oral gavage
Duration of test:	4 weeks
Doses:	0, 25, 150, or 1000 mg/kg./day
Sex:	Males and females
Exposure period:	4 weeks
Frequency of treatment:	Once daily, 7 days/week
Control group and treatment:	Concurrent vehicle control (corn oil)
Post exposure observation period:	None
Statistical methods:	Analysis of variance (Snedecor and Cochran, 1980) Kruskal-Wallis non-parametric analysis (Hollander and Wolfe, 1973) Fisher's Exact Probability test (Siegel 1956)
Test Conditions:	Groups of ten rats (5M:5F) were dosed orally by gavage once daily over a period of 28 days. Animals were approximately 41 days old on the first day of dosing. Animals were regularly monitored for any signs of ill health or reaction to treatment. Detailed functional observations were performed weekly, with additional functional observations performed during pretrial and week four. Body weights and food consumption were recorded twice weekly. Blood and urine samples were collected during week four of the study. After four weeks of treatment, animals were sacrificed and subjected to necropsy. A comprehensive list of organs were weighed and /or preserved (adrenal, brain, epididymis, eye, gastrointestinal tract including stomach, duodenum, jejunum, ileum, caecum, colon, rectum, heart, kidney, liver, lung, bone marrow, mesenteric lymph node, ovary, pituitary, prostate, sciatic nerve, spinal cord, spleen,

submandibular lymph node, testis, thymus, thyroid with parathyroid, trachea, urinary bladder, uterus). Tissues from the controls and high dose animals were subjected to histological examination. Histology was also performed on the male kidneys from the lower doses.

Results

NOAEL (NOEL): The NOEL for reproductive effects from limited data (effect on reproductive organs) appears to be 1000 mg/kg/day (the highest dose tested).

Actual dose received by dose level by sex if known: Actual doses for both sexes were 0, 25, 150, or 1000 mg/kg/day

Remarks: Please see Repeated Dose Toxicity, Section 5.5 A for general toxicity results. There was no evidence of toxicity to reproductive organs in animals treated at levels up to 1000 mg/kg/day.

Reliability: (1) Reliable without restrictions.

References: Clubb, S. (2000) AmoDrill 1000 4-Week Toxicity Study Including Neurotoxicity Screening in Rats with Administration by Gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE Scotland. Sponsor Amoco Corporation (unpublished report).

(3) Test Substance

Identity (purity): CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only)
(<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)

Method

Method/guideline: OECD 408 See Section 5.5 B for general toxicity endpoints)
Test type: Subchronic Oral Toxicity - Rodent: 90-day Study
GLP: Yes
Year: 1999
Species: Rat
Strain: Crl:CD BR
Route of Administration: Oral gavage

Duration of test: 17 weeks
Doses: 0, 100, 500, and 1000 mg/kg /day
Sex: Males and females

Exposure period:	13 weeks
Frequency of treatment:	Once daily
Control group and treatment:	Concurrent vehicle control (corn oil)
Post exposure observation period:	4 weeks
Statistical methods:	See Section 5.5.B
Test Conditions:	See Section 5.5.B
Results	
NOAEL (NOEL):	The NOEL for reproductive effects from limited data (effect on reproductive organs) appears to be 1000 mg/kg/day (the highest dose tested)
Actual dose received by dose level by sex if known:	The mean concentration of C20-24 alkenes, branched and linear, in test formulations analyzed during the study were within ± 12% of nominal concentrations, confirming the accuracy of formulation.
Remarks:	Please see Repeated Dose Toxicity, Section 5.5 B for general toxicity results. There was no evidence of toxicity to reproductive organs in animals treated at levels up to 1000 mg/kg/day.
Reliability:	(1) Reliable without restrictions.
References:	Brooker AJ (1999). C20-24 Alkenes, branched and linear: Toxicity Study By Oral Gavage Administration to CD Rats for 13 Weeks Followed by a 4-Week Recovery Period. Project Nos. CHR/052 and CHR/053. Conducted by Huntingdon Life Sciences for Chevron Research and Technology Company (unpublished report).

B. Developmental Toxicity

Test Substance

Identity (purity):	CAS 27070-58-2, Octadecenes; CAS 182636-02-8, Branched Octadecenes

Remarks:	Test substance identified as Octadecene C18 Compound; 96.7% C18 olefins; 1.84% C16 olefins, 0.95% C20 olefins; 3.30% normal alpha olefins; 32.5% methyl branched isomers; 67.5% linear olefins.
Method/guideline:	OECD 421 (see Section 5.9.A(1) for reproductive toxicity endpoints)
Type:	Reproduction/Developmental Toxicity Screening Test
GLP:	Yes
Year:	2003
Species:	Rat
Strain:	Sprague-Dawley
Route of administration:	Oral gavage
Concentration levels:	0, 100, 500 and 1000 mg/kg/day
Sex:	Male and female
Control group and treatment:	Corn oil by oral gavage (5 mL/kg)
Frequency of treatment:	Daily
Duration of test:	Through lactation day 4 for pups
Premating exposure period for males:	Two weeks
Premating exposure period for females:	Two weeks
Statistical methods:	Data, including body weights, body weight changes, food consumption, implantation sites, corpora lutea, gestation length and mean live litter size, were analyzed by ANOVA. If significance was observed with ANOVA, control to treatment group comparisons were performed using Dunnett's test. Count data were analyzed using R x C Chi-Square test followed by Fisher's Exact Test for copulation and fertility indices, pup sex ratios, the number of live and dead pups per group (on lactation day 0) and pup survival (after lactation day 0). Absolute and relative organ weights were analyzed for homogeneity of variance using Bartlett's test. If significance was detected with Bartlett's test ($p<0.01$), multiple group comparisons proceeded using the Kruskal-Wallis non-parametric ANOVA, followed by Dunn's test, when $p<0.05$. If significance was not detected with Bartlett's test, parametric procedures were used to analyze the data, i.e., ANOVA followed by Dunnett's test when $p<0.05$. All statistical analyses were performed using the SLI Alpha ReproTox computer system (version 1.5.3 or later). All analyses were two-tailed with a minimum significance level of 5% ($p<0.05$).
Test Conditions:	The study consisted of a vehicle control and three treatment groups, with 12 males and 12 females in each group. Octadecenes C18 Compound was dissolved in corn oil and administered at dosage levels of 100, 500 and 1000 mg/kg/day, once daily by oral gavage, to F0 parental animals. All doses were given at a constant volume of 5 mL/kg. Control animals were administered corn oil under the same experimental conditions at an equivalent dose volume. F0 males were treated for two weeks prior to mating, during mating and four weeks following mating. F0 females were treated for two weeks prior to mating, during mating, during gestation and following parturition. Males and females were dosed up to

and including the day prior to scheduled euthanasia. See Section 5.9.A.(1) for additional details.

Results

NOAEL:	NOAEL for maternal toxicity = 1000 mg/kg/day NOAEL for developmental toxicity = 1000 mg/kg/day
Actual dose received by dose level by sex if known:	All dosing formulations were found to be within 20% of the stated concentration.
Maternal and Paternal general toxicity:	No toxicologically meaningful effects seen at 1000 mg/kg/day (see Section 5.9.A.(1) for details)
Remarks:	The mean number of F0 implantation sites and corpora lutea, the mean number of F1 pups delivered, the live birth and viability indices, and the mean live pups per litter and pup sex ratio on lactation days 0 and 4 were comparable between the control and test article-treated groups. No remarkable findings were noted in the pups during lactation days 0-4. There were no statistically significant or toxicologically meaningful differences in mean pup weights in the test article-treated groups compared to controls on lactation days 1 and 4. No remarkable gross necropsy findings were noted for pups found dead, euthanized for cause or euthanized on lactation day 4. Based on the results of this study, a dosage level of 1000 mg/kg/day was considered a no-observed-adverse-effect level (NOAEL) for developmental effects.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Thorsrud, B.A. (2003) An oral (gavage) reproduction/developmental toxicity screening study in Sprague Dawley rats with (C18) Octadecenes. Report No. 3604.1. Conducted by Springborn Laboratories, Spencerville, OH, for American Chemistry Council Higher Olefins Panel (unpublished study).

5.10 Other Relevant Information

A. Aspiration

Test Substance

Identity:	CAS No. 112-88-9, 1-Octadecene

Method

Type:	General toxicity – aspiration
Species:	Rat
Strain:	Wistar
Sex:	Male
Route of Administration:	aspiration
Dose:	0.2 mL

Results: See Remarks

Remarks: C6-C18 alkenes (even carbon numbers, alpha olefins), source and purity unspecified, were assessed for aspiration hazard in an animal study using Wistar rats. Four or five males were used per test article. Two-tenths mL of the test material was placed in the mouths of rats that had been anesthetized to the point of apnea in a covered wide mouth gallon jar containing about 1 inch of wood shavings moistened with approximately 1 ounce of anhydrous diethyl ether. As the animals began to breathe again, the nostrils were held until the test material had been aspirated or the animal regained consciousness. All alkenes tested except 1- hexene were aspirated into the lungs. 1-Hexene was difficult to dose because of its volatility. Two animals survived because the hydrocarbon "boiled" out of the mouth before it was aspirated. All animals exposed to C_8 to C_{14} died within 24 hours. With C_{16} and C_{18}, there was only one death (C_{18}). Lung weights were increased in alkenes-treated animals compared with controls. The affected animals showed chemical pneumonitis. The report concluded that there is a significant aspiration hazard with C_6 to C_{14} alkenes.

Reference: Gerarde, H.W. (1963) Toxicological Studies on Hydrocarbons. Archives of Environmental Health, 6:329-341.

B. Neurotoxicity

(1) Test Substance

Identity (purity):	C16/18 isomerised olefin
Remarks:	C14-0.4%, C16-53.6%, C18-37.6%, C20-7.9%, C22-0.5%. Linear terminal 1.8%, linear internal 71.9%, Branched terminal 15.6% Trisubstituted 10.7%.

Method

Method/guideline:	OECD 407 (see Sec. 5.5.A for general toxicity endpoints)
Test type:	subacute toxicity
GLP:	Yes
Year:	2000
Species:	Rat
Strain:	Sprague Dawley (crl:CD BR)
Route of	

Administration:	Oral gavage
Duration of test:	4 weeks
Doses:	0, 25, 150, or 1000 mg/kg./day
Sex:	Males and females
Exposure period:	4 weeks
Frequency of treatment:	Once daily, 7 days/week
Control group and treatment:	Concurrent vehicle control (corn oil)
Post exposure observation period:	None
Statistical methods:	Analysis of variance (Snedecor and Cochran, 1980) Kruskal-Wallis non-parametric analysis (Hollander and Wolfe, 1973) Fisher's Exact Probability test (Siegel 1956)
Test Conditions:	See Section 5.5.A
Results	
NOAEL (NOEL):	NOAEL = 1000 mg/kg/day (neurotoxicity)
Actual dose received by dose level by sex if known:	Actual doses for both sexes were 0, 25, 150, or 1000 mg/kg/day.
Remarks:	See Sec. 5.5.A for general toxicity results. There was no evidence of neurotoxicity noted in animals treated at levels up to 1000 mg/kg/day.
Reliability:	(1) Reliable without restrictions.
Flag:	Key study for SIDS endpoint.
References:	Clubb, S. (2000) AmoDrill 1000 4-Week Toxicity Study Including Neurotoxicity Screening in Rats with Administration by Gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE Scotland. Sponsor Amoco Corporation (unpublished report).

(2) Test Substance

Identity (purity):	CAS Nos. C20=182636-03-9, C22=182636-04-0, C24=182636-05-1; C20-24 Alkenes, Branched and Linear (even-numbered carbons only)

	(<1% C18's, 40-44% C20's, 35-39% C22's, 18-22% C24's, <1% C26's; >70% branched)
Method	
Method/guideline:	OECD 408 (see Sec. 5.5.B for general toxicity endpoints)
Test type:	Subchronic Oral Toxicity - Rodent: 90-day Study
GLP:	Yes
Year:	1999
Species:	Rat
Strain:	Crl:CD BR
Route of Administration:	Oral gavage
Duration of test:	17 weeks
Doses:	0, 100, 500, and 1000 mg/kg /day
Sex:	Males and females
Exposure period:	13 weeks
Frequency of treatment:	Once daily
Control group and treatment:	Concurrent vehicle control (corn oil)
Post exposure observation period:	4 weeks
Statistical methods:	See Section 5.5.B
Test Conditions:	See Section 5.5.B
Results	
NOAEL (NOEL):	1000 mg/kg/day (neurotoxicity)
Actual dose received by dose level by sex if known:	The mean concentration of C20-24 alkenes, branched and linear, in test formulations analyzed during the study were within ± 12% of nominal concentrations, confirming the accuracy of formulation.
Remarks:	See Sec. 5.5.B for general toxicity results. In the 13-wk study, no neurobehavioral effects were noted.
Reliability:	(1) Reliable without restrictions.
Flag:	Key study for SIDS endpoint.

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5.11 Experience with Human Exposure

No data available

6.0 References

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